



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 05:16 PM UTC

PDB ID : 9B4G / pdb_00009b4g
EMDB ID : EMD-44180
Title : Structure of inhibitor-bound human PSS1
Authors : Long, T.; Li, X.
Deposited on : 2024-03-20
Resolution : 2.87 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

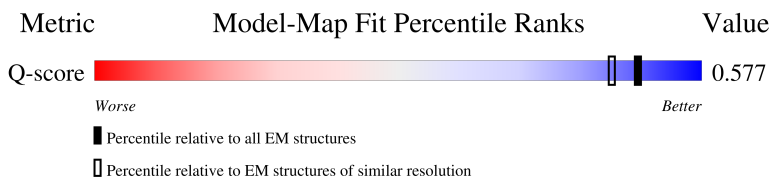
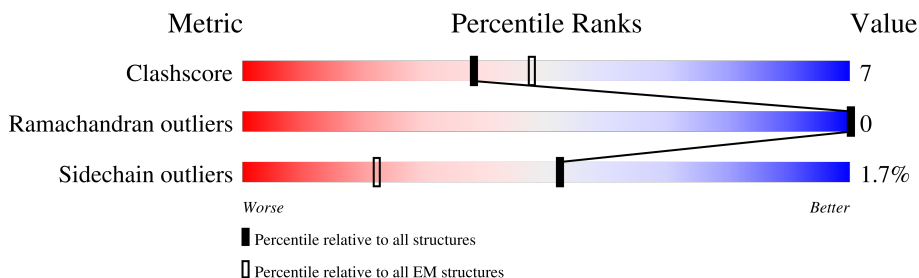
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	409	 78% 16% • 5%
1	B	409	 78% 16% • 5%

2 Entry composition [i](#)

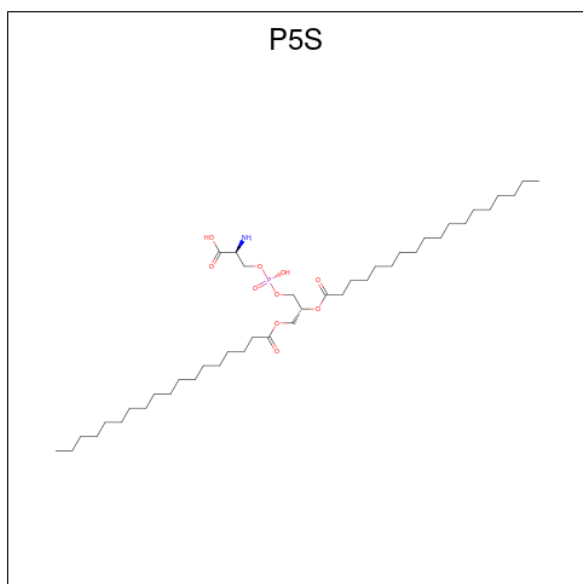
There are 8 unique types of molecules in this entry. The entry contains 7065 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphatidylserine synthase 1.

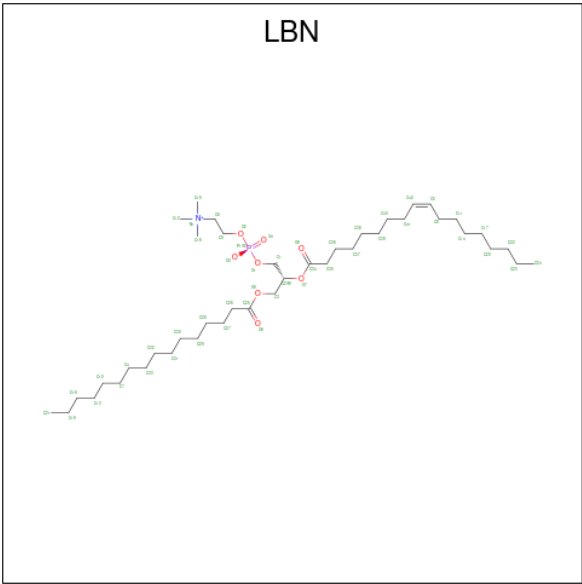
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	388	Total	C	N	O	S	0	0
			3238	2180	514	523	21		
1	B	388	Total	C	N	O	S	0	0
			3233	2177	513	522	21		

- Molecule 2 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



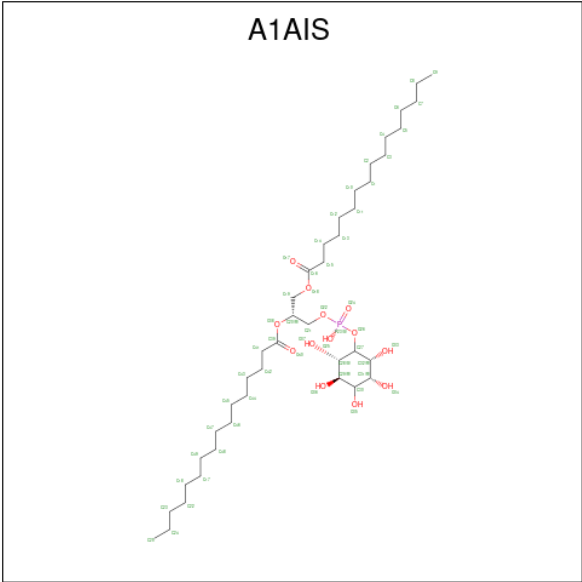
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			43	31	1	10	1	
2	A	1	Total	C	N	O	P	0
			31	19	1	10	1	
2	B	1	Total	C	N	O	P	0
			43	31	1	10	1	
2	B	1	Total	C	N	O	P	0
			31	19	1	10	1	

- Molecule 3 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: C₄₂H₈₂NO₈P).



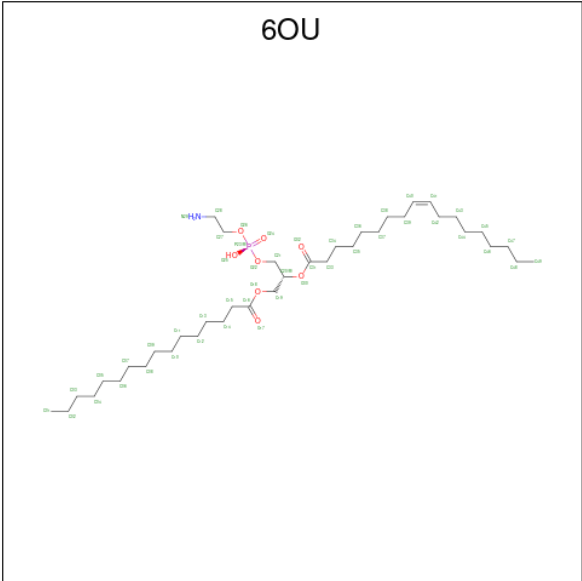
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 4 is (2R)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl dihexadecanoate (CCD ID: A1AIS) (formula: C₄₁H₇₉O₁₃P).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			40	26	13	1	
4	B	1	Total	C	O	P	0
			40	26	13	1	

- Molecule 5 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			42	32	1	8	1	

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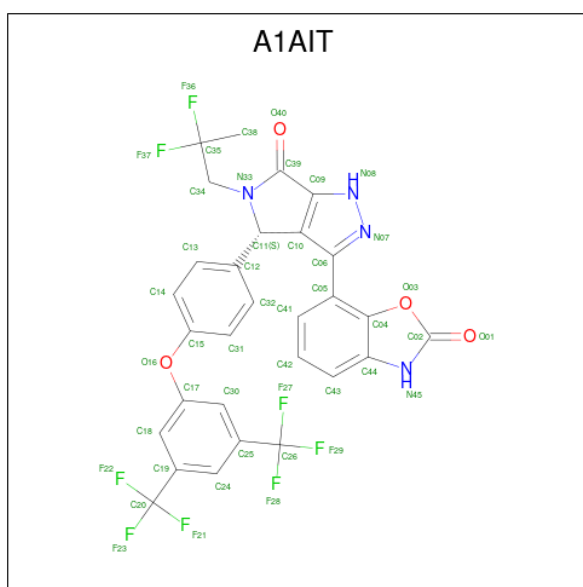
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Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	

- Molecule 7 is (7P)-7-[(4S)-4-{4-[3,5-bis(trifluoromethyl)phenoxy]phenyl}-5-(2,2-difluoropropyl)-6-oxo-1,4,5,6-tetrahydropyrrolo[3,4-c]pyrazol-3-yl]-1,3-benzoxazol-2(3H)-one (CCD ID: A1AIT) (formula: C₂₉H₁₈F₈N₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	F	N	O	0
			45	29	8	4	4	
7	B	1	Total	C	F	N	O	0
			45	29	8	4	4	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	7	Total	O	0
			7	7	

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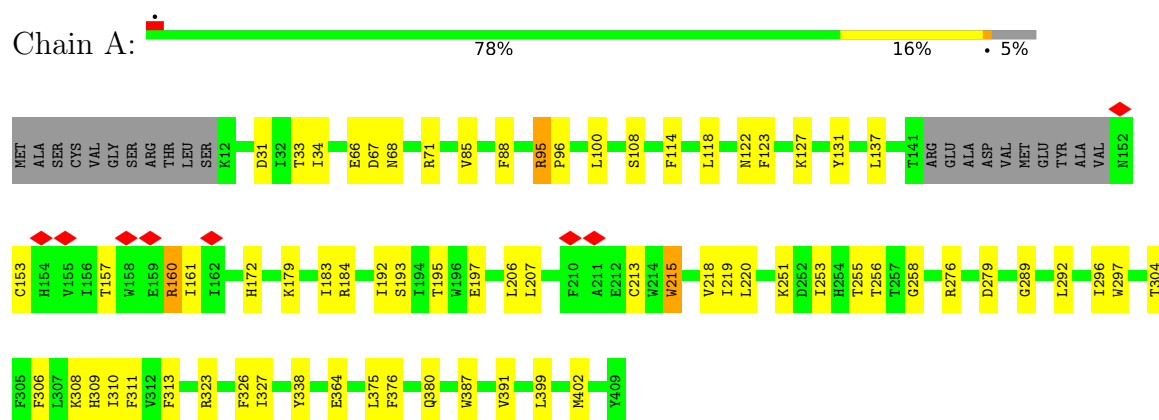
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Mol	Chain	Residues	Atoms		AltConf
8	B	7	Total	O	0
			7	7	

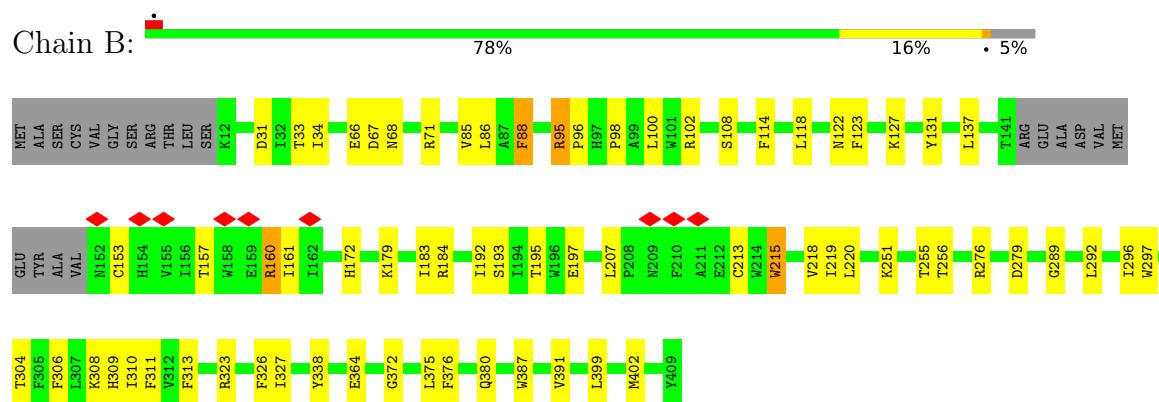
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phosphatidylserine synthase 1



• Molecule 1: Phosphatidylserine synthase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	271650	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.431	Depositor
Minimum map value	-2.252	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.312	Depositor
Map size ($\text{\AA}$)	250.29, 250.29, 250.29	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8343, 0.8343, 0.8343	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LBN, A1AIT, P5S, A1AIS, 6OU, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/3352	0.37	0/4567
1	B	0.20	0/3346	0.37	0/4558
All	All	0.20	0/6698	0.37	0/9125

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3238	0	3185	50	0
1	B	3233	0	3175	52	0
2	A	74	0	80	3	0
2	B	74	0	80	2	0
3	A	88	0	0	0	0
3	B	88	0	0	0	0
4	A	40	0	0	0	0
4	B	40	0	0	1	0
5	A	42	0	0	1	0
5	B	42	0	0	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	45	0	0	0	0
7	B	45	0	0	0	0
8	A	7	0	0	0	0
8	B	7	0	0	0	0
All	All	7065	0	6520	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HG2	1:A:311:PHE:CE1	1.60	1.36
1:B:127:LYS:HG2	1:B:311:PHE:CE1	1.60	1.34
1:B:127:LYS:CG	1:B:311:PHE:HE1	1.67	1.06
1:A:127:LYS:CG	1:A:311:PHE:HE1	1.67	1.05
1:A:114:PHE:CE2	1:A:118:LEU:HD11	1.95	1.02
1:B:114:PHE:CE2	1:B:118:LEU:HD11	1.95	1.02
1:B:387:TRP:O	1:B:391:VAL:HG23	1.94	0.68
1:A:195:THR:CG2	1:A:391:VAL:HG13	2.24	0.68
1:B:195:THR:CG2	1:B:391:VAL:HG13	2.24	0.68
1:A:387:TRP:O	1:A:391:VAL:HG23	1.93	0.68
1:B:153:CYS:SG	1:B:213:CYS:N	2.71	0.63
1:B:161:ILE:HG23	1:B:220:LEU:HD21	1.80	0.63
1:A:153:CYS:SG	1:A:213:CYS:N	2.71	0.63
1:A:161:ILE:HG23	1:A:220:LEU:HD21	1.80	0.62
1:B:207:LEU:HD13	1:B:309:HIS:HD2	1.64	0.62
1:A:207:LEU:HD13	1:A:309:HIS:HD2	1.65	0.62
1:B:207:LEU:CD1	1:B:309:HIS:CD2	2.85	0.60
1:B:207:LEU:HD13	1:B:309:HIS:CD2	2.37	0.60
1:A:207:LEU:CD1	1:A:309:HIS:CD2	2.85	0.59
1:B:123:PHE:HE1	1:B:311:PHE:CZ	2.21	0.59
1:B:306:PHE:O	1:B:310:ILE:HG12	2.02	0.59
1:B:31:ASP:O	2:B:603:P5S:N	2.36	0.59
1:A:123:PHE:HE1	1:A:311:PHE:CZ	2.21	0.59
1:A:306:PHE:O	1:A:310:ILE:HG12	2.02	0.58
1:A:207:LEU:HD13	1:A:309:HIS:CD2	2.37	0.58
1:B:207:LEU:HD21	1:B:375:LEU:HD22	1.86	0.58
1:A:31:ASP:O	2:A:502:P5S:N	2.36	0.58
1:A:127:LYS:CG	1:A:311:PHE:CE1	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LYS:CG	1:B:311:PHE:CE1	2.57	0.57
1:A:207:LEU:HD21	1:A:375:LEU:HD22	1.86	0.57
1:B:127:LYS:HG2	1:B:311:PHE:HE1	0.70	0.57
1:B:276:ARG:HH21	1:B:279:ASP:HA	1.70	0.57
1:A:276:ARG:HH21	1:A:279:ASP:HA	1.70	0.56
1:B:195:THR:HG21	1:B:391:VAL:HG13	1.90	0.54
1:A:195:THR:HG21	1:A:391:VAL:HG13	1.90	0.53
1:A:127:LYS:HG2	1:A:311:PHE:HE1	0.70	0.53
1:A:289:GLY:O	1:A:338:TYR:OH	2.26	0.52
1:B:289:GLY:O	1:B:338:TYR:OH	2.26	0.52
1:A:292:LEU:O	1:A:296:ILE:HG12	2.11	0.50
1:A:308:LYS:NZ	1:A:313:PHE:O	2.45	0.50
1:B:114:PHE:O	1:B:118:LEU:HG	2.12	0.50
1:B:292:LEU:O	1:B:296:ILE:HG12	2.11	0.49
1:B:308:LYS:NZ	1:B:313:PHE:O	2.45	0.49
1:A:213:CYS:HB3	1:A:215:TRP:CZ3	2.48	0.49
1:B:172:HIS:NE2	5:B:606:6OU:O22	2.46	0.49
1:A:218:VAL:HG23	1:A:219:ILE:HG13	1.94	0.49
1:B:213:CYS:HB3	1:B:215:TRP:CZ3	2.48	0.49
1:A:172:HIS:NE2	5:A:505:6OU:O22	2.46	0.48
1:B:218:VAL:HG23	1:B:219:ILE:HG13	1.94	0.48
1:A:114:PHE:O	1:A:118:LEU:HG	2.12	0.48
1:B:123:PHE:CE1	1:B:311:PHE:CZ	3.02	0.48
1:A:123:PHE:CE1	1:A:311:PHE:CZ	3.01	0.47
1:B:255:THR:OG1	1:B:256:THR:N	2.48	0.47
1:B:213:CYS:HB3	1:B:215:TRP:HZ3	1.79	0.47
1:B:304:THR:OG1	1:B:323:ARG:NH1	2.43	0.47
1:A:376:PHE:HB3	1:A:380:GLN:HB2	1.96	0.47
1:B:34:ILE:HG12	1:B:251:LYS:HE3	1.97	0.47
1:A:323:ARG:NH2	1:A:364:GLU:OE2	2.48	0.47
1:B:96:PRO:HD2	1:B:100:LEU:HD12	1.97	0.46
1:A:34:ILE:HG12	1:A:251:LYS:HE3	1.97	0.46
1:B:376:PHE:HB3	1:B:380:GLN:HB2	1.96	0.46
1:A:213:CYS:HB3	1:A:215:TRP:HZ3	1.79	0.46
1:B:192:ILE:HG13	1:B:297:TRP:CE3	2.51	0.46
1:A:192:ILE:HG13	1:A:297:TRP:CE3	2.51	0.46
1:B:108:SER:HA	1:B:326:PHE:HZ	1.81	0.45
1:A:96:PRO:HD2	1:A:100:LEU:HD12	1.97	0.45
1:A:33:THR:OG1	2:A:502:P5S:O13	2.35	0.45
1:A:108:SER:HA	1:A:326:PHE:HZ	1.81	0.45
1:A:255:THR:OG1	1:A:256:THR:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:OG1	1:A:323:ARG:NH1	2.43	0.45
1:A:68:ASN:ND2	1:B:122:ASN:HD22	2.16	0.44
1:A:179:LYS:O	1:A:183:ILE:HG12	2.18	0.44
1:B:114:PHE:CZ	1:B:118:LEU:HD11	2.50	0.43
1:B:179:LYS:O	1:B:183:ILE:HG12	2.18	0.43
1:B:33:THR:OG1	2:B:603:P5S:O13	2.35	0.43
1:B:131:TYR:CD1	1:B:137:LEU:HD23	2.54	0.43
1:B:323:ARG:NH2	1:B:364:GLU:OE2	2.48	0.43
1:A:122:ASN:HD22	1:B:68:ASN:ND2	2.16	0.42
1:A:131:TYR:CD1	1:A:137:LEU:HD23	2.54	0.42
1:B:95:ARG:HG3	1:B:96:PRO:HA	2.01	0.42
1:A:95:ARG:HG3	1:A:96:PRO:HA	2.01	0.42
1:A:323:ARG:O	1:A:327:ILE:HG12	2.20	0.41
1:A:114:PHE:CZ	1:A:118:LEU:HD11	2.50	0.41
1:A:193:SER:O	1:A:197:GLU:HG2	2.20	0.41
1:B:323:ARG:O	1:B:327:ILE:HG12	2.20	0.41
1:B:193:SER:O	1:B:197:GLU:HG2	2.20	0.41
1:A:67:ASP:O	1:A:71:ARG:HG2	2.21	0.41
1:A:157:THR:O	1:A:160:ARG:HG3	2.21	0.41
1:A:399:LEU:HA	1:A:402:MET:HE3	2.02	0.41
1:B:157:THR:O	1:B:160:ARG:HG3	2.21	0.41
1:B:67:ASP:O	1:B:71:ARG:HG2	2.21	0.41
1:A:206:LEU:HA	1:A:206:LEU:HD12	1.89	0.40
1:A:253:ILE:HG21	1:A:258:GLY:C	2.46	0.40
1:B:66:GLU:H	1:B:66:GLU:CD	2.29	0.40
1:B:399:LEU:HA	1:B:402:MET:HE3	2.02	0.40
1:B:86:LEU:O	4:B:605:A1AIS:O33	2.40	0.40
1:B:98:PRO:O	1:B:102:ARG:HG3	2.21	0.40
1:A:66:GLU:CD	1:A:66:GLU:H	2.29	0.40
2:A:502:P5S:H20A	2:A:502:P5S:H23	2.00	0.40
1:B:88:PHE:HD1	1:B:88:PHE:HA	1.73	0.40
1:B:310:ILE:HD12	1:B:372:GLY:HA2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/409 (94%)	375 (98%)	9 (2%)	0	100	100
1	B	384/409 (94%)	375 (98%)	9 (2%)	0	100	100
All	All	768/818 (94%)	750 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/367 (94%)	338 (98%)	6 (2%)	53	80
1	B	342/367 (93%)	336 (98%)	6 (2%)	51	78
All	All	686/734 (94%)	674 (98%)	12 (2%)	52	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	A	88	PHE
1	A	95	ARG
1	A	160	ARG
1	A	184	ARG
1	A	215	TRP
1	B	85	VAL
1	B	88	PHE
1	B	95	ARG
1	B	160	ARG
1	B	184	ARG
1	B	215	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	298	GLN
1	A	309	HIS
1	B	122	ASN
1	B	205	HIS
1	B	246	HIS
1	B	298	GLN
1	B	309	HIS
1	B	380	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	P5S	B	602	-	41,42,53	1.21	3 (7%)	43,49,60	1.05	2 (4%)
3	LBN	A	508	-	35,35,51	1.28	4 (11%)	41,43,59	1.06	2 (4%)
5	6OU	A	505	-	41,41,48	1.09	4 (9%)	44,46,53	1.02	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1AIS	B	605	-	40,40,55	1.05	4 (10%)	49,52,67	1.31	6 (12%)
2	P5S	A	502	-	29,30,53	1.37	3 (10%)	31,37,60	1.07	2 (6%)
5	6OU	B	606	-	41,41,48	1.10	4 (9%)	44,46,53	1.02	2 (4%)
7	A1AIT	A	507	-	48,50,50	1.99	9 (18%)	68,79,79	1.78	12 (17%)
3	LBN	B	601	-	35,35,51	1.28	4 (11%)	41,43,59	1.06	2 (4%)
7	A1AIT	B	608	-	48,50,50	1.99	9 (18%)	68,79,79	1.79	12 (17%)
4	A1AIS	A	504	-	40,40,55	1.05	3 (7%)	49,52,67	1.31	6 (12%)
2	P5S	B	603	-	29,30,53	1.37	3 (10%)	31,37,60	1.07	2 (6%)
3	LBN	B	604	-	51,51,51	1.09	4 (7%)	57,59,59	0.84	2 (3%)
2	P5S	A	501	-	41,42,53	1.21	3 (7%)	43,49,60	1.05	2 (4%)
3	LBN	A	503	-	51,51,51	1.09	4 (7%)	57,59,59	0.84	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P5S	B	602	-	-	25/48/48/59	-
3	LBN	A	508	-	-	21/39/39/55	-
5	6OU	A	505	-	-	25/45/45/52	-
4	A1AIS	B	605	-	-	17/35/59/74	0/1/1/1
2	P5S	A	502	-	-	19/36/36/59	-
5	6OU	B	606	-	-	25/45/45/52	-
7	A1AIT	A	507	-	-	2/29/45/45	0/6/6/6
3	LBN	B	601	-	-	21/39/39/55	-
7	A1AIT	B	608	-	-	2/29/45/45	0/6/6/6
4	A1AIS	A	504	-	-	17/35/59/74	0/1/1/1
2	P5S	B	603	-	-	19/36/36/59	-
3	LBN	B	604	-	-	30/55/55/55	-
2	P5S	A	501	-	-	25/48/48/59	-
3	LBN	A	503	-	-	30/55/55/55	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	507	A1AIT	C02-N45	8.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	608	A1AIT	C02-N45	8.05	1.42	1.35
7	A	507	A1AIT	C39-N33	6.69	1.44	1.35
7	B	608	A1AIT	C39-N33	6.69	1.44	1.35
7	A	507	A1AIT	O03-C04	3.98	1.45	1.38
7	B	608	A1AIT	O03-C04	3.98	1.45	1.38
2	A	502	P5S	O19-C17	3.48	1.43	1.33
2	B	603	P5S	O19-C17	3.48	1.43	1.33
2	A	501	P5S	O19-C17	3.27	1.42	1.33
2	B	602	P5S	O19-C17	3.27	1.42	1.33
2	A	501	P5S	O37-C38	3.09	1.43	1.34
2	B	602	P5S	O37-C38	3.09	1.43	1.34
2	B	603	P5S	O37-C38	3.07	1.43	1.34
7	A	507	A1AIT	C44-N45	3.07	1.44	1.38
7	B	608	A1AIT	C44-N45	3.07	1.44	1.38
3	A	503	LBN	O7-C34	3.07	1.42	1.34
3	B	604	LBN	O7-C34	3.07	1.42	1.34
2	A	502	P5S	O37-C38	3.06	1.42	1.34
5	A	505	6OU	O18-C16	3.06	1.42	1.33
5	B	606	6OU	O18-C16	3.06	1.42	1.33
3	B	601	LBN	O7-C34	3.05	1.42	1.34
3	A	508	LBN	O7-C34	3.04	1.42	1.34
7	A	507	A1AIT	C11-N33	-3.02	1.43	1.47
7	B	608	A1AIT	C11-N33	-3.02	1.43	1.47
4	A	504	A1AIS	O38-C20	-2.85	1.39	1.46
4	B	605	A1AIS	O38-C20	-2.85	1.39	1.46
5	A	505	6OU	O30-C20	-2.75	1.40	1.46
5	B	606	6OU	O30-C20	-2.75	1.40	1.46
3	A	508	LBN	O5-C25	2.58	1.40	1.33
3	B	601	LBN	O5-C25	2.58	1.40	1.33
3	A	503	LBN	O5-C25	2.48	1.40	1.33
3	B	604	LBN	O5-C25	2.48	1.40	1.33
7	A	507	A1AIT	C09-N08	-2.47	1.32	1.35
7	B	608	A1AIT	C09-N08	-2.47	1.32	1.35
5	B	606	6OU	O30-C31	2.45	1.41	1.34
7	A	507	A1AIT	C05-C06	2.42	1.52	1.48
7	B	608	A1AIT	C05-C06	2.42	1.52	1.48
5	A	505	6OU	O30-C31	2.41	1.41	1.34
2	A	501	P5S	O37-C2	-2.31	1.41	1.46
2	B	602	P5S	O37-C2	-2.31	1.41	1.46
4	A	504	A1AIS	O18-C19	-2.30	1.40	1.45
4	B	605	A1AIS	O18-C19	-2.30	1.40	1.45
2	A	502	P5S	O37-C2	-2.25	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	603	P5S	O37-C2	-2.25	1.41	1.46
7	A	507	A1AIT	O40-C39	-2.21	1.18	1.23
3	A	508	LBN	C6-N1	-2.20	1.44	1.51
3	B	601	LBN	C6-N1	-2.20	1.44	1.51
7	B	608	A1AIT	O40-C39	-2.18	1.18	1.23
3	B	604	LBN	O5-C3	-2.17	1.40	1.45
5	B	606	6OU	P23-O22	2.16	1.67	1.59
3	A	503	LBN	O5-C3	-2.15	1.40	1.45
5	A	505	6OU	P23-O22	2.15	1.67	1.59
4	A	504	A1AIS	O18-C16	2.15	1.39	1.33
4	B	605	A1AIS	O18-C16	2.15	1.39	1.33
3	A	503	LBN	O7-C2	-2.15	1.41	1.46
3	B	604	LBN	O7-C2	-2.15	1.41	1.46
7	A	507	A1AIT	O03-C02	2.08	1.40	1.38
7	B	608	A1AIT	O03-C02	2.08	1.40	1.38
3	B	601	LBN	O7-C2	-2.07	1.41	1.46
3	A	508	LBN	O7-C2	-2.06	1.41	1.46
4	B	605	A1AIS	P23-O26	2.01	1.65	1.59

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	507	A1AIT	C11-N33-C39	-6.60	108.44	113.47
7	B	608	A1AIT	C11-N33-C39	-6.60	108.44	113.47
7	A	507	A1AIT	C10-C11-N33	6.18	107.62	101.36
7	B	608	A1AIT	C10-C11-N33	6.18	107.62	101.36
4	A	504	A1AIS	O38-C39-C41	4.42	121.05	111.48
4	B	605	A1AIS	O38-C39-C41	4.42	121.05	111.48
5	A	505	6OU	O30-C31-C33	4.40	121.00	111.48
5	B	606	6OU	O30-C31-C33	4.40	121.00	111.48
2	A	501	P5S	O37-C38-C39	4.05	120.24	111.48
2	B	602	P5S	O37-C38-C39	4.05	120.24	111.48
3	A	508	LBN	O7-C34-C35	4.05	120.23	111.48
3	B	601	LBN	O7-C34-C35	4.03	120.20	111.48
4	A	504	A1AIS	C31-C32-C27	3.57	117.77	109.68
4	B	605	A1AIS	C31-C32-C27	3.57	117.77	109.68
2	B	603	P5S	O37-C38-C39	3.51	119.07	111.48
2	A	502	P5S	O37-C38-C39	3.49	119.03	111.48
3	A	503	LBN	O7-C34-C35	3.43	118.89	111.48
3	B	604	LBN	O7-C34-C35	3.43	118.89	111.48
7	A	507	A1AIT	C44-N45-C02	-3.26	108.14	109.90
7	B	608	A1AIT	C44-N45-C02	-3.26	108.14	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	A1AIS	C32-C31-C30	3.15	116.37	110.83
4	B	605	A1AIS	C32-C31-C30	3.15	116.37	110.83
7	A	507	A1AIT	O03-C04-C05	3.15	131.58	125.70
7	B	608	A1AIT	O03-C04-C05	3.15	131.58	125.70
2	A	502	P5S	O19-C17-C20	3.02	121.03	111.83
2	B	603	P5S	O19-C17-C20	3.02	121.03	111.83
7	A	507	A1AIT	C04-C05-C06	-2.95	117.74	122.78
7	B	608	A1AIT	C04-C05-C06	-2.95	117.74	122.78
7	B	608	A1AIT	O03-C02-O01	2.93	125.97	121.98
7	A	507	A1AIT	O03-C02-O01	2.90	125.94	121.98
2	B	602	P5S	O19-C17-C20	2.90	120.69	111.83
5	A	505	6OU	O18-C16-C15	2.89	120.66	111.83
5	B	606	6OU	O18-C16-C15	2.89	120.66	111.83
2	A	501	P5S	O19-C17-C20	2.89	120.66	111.83
7	A	507	A1AIT	C12-C11-C10	-2.86	108.97	114.02
7	B	608	A1AIT	C12-C11-C10	-2.86	108.98	114.02
4	B	605	A1AIS	C32-C27-C28	2.81	114.76	110.86
3	A	503	LBN	O5-C25-C26	2.81	120.40	111.83
3	B	604	LBN	O5-C25-C26	2.81	120.40	111.83
4	A	504	A1AIS	C32-C27-C28	2.80	114.74	110.86
3	A	508	LBN	O5-C25-C26	2.69	120.04	111.83
3	B	601	LBN	O5-C25-C26	2.69	120.04	111.83
7	B	608	A1AIT	O01-C02-N45	-2.67	126.18	129.81
7	A	507	A1AIT	O01-C02-N45	-2.64	126.21	129.81
4	A	504	A1AIS	O18-C16-C15	2.58	119.70	111.83
4	B	605	A1AIS	O18-C16-C15	2.58	119.70	111.83
7	A	507	A1AIT	C04-C44-N45	2.58	107.78	105.64
7	B	608	A1AIT	C04-C44-N45	2.58	107.78	105.64
7	A	507	A1AIT	C04-O03-C02	2.40	107.95	107.13
7	B	608	A1AIT	C04-O03-C02	2.40	107.95	107.13
7	B	608	A1AIT	C32-C12-C11	-2.39	117.20	120.69
7	A	507	A1AIT	C32-C12-C11	-2.37	117.22	120.69
4	A	504	A1AIS	C20-O38-C39	-2.21	112.50	117.80
4	B	605	A1AIS	C20-O38-C39	-2.21	112.50	117.80
7	A	507	A1AIT	C09-C10-C06	2.16	106.50	104.86
7	B	608	A1AIT	C09-C10-C06	2.16	106.50	104.86

There are no chirality outliers.

All (278) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	P5S	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	A	502	P5S	OXT-C-CA-CB
2	A	502	P5S	C3-O16-P12-OG
2	A	502	P5S	C3-O16-P12-O13
2	A	502	P5S	C3-O16-P12-O15
2	B	603	P5S	O-C-CA-CB
2	B	603	P5S	OXT-C-CA-CB
2	B	603	P5S	C3-O16-P12-OG
2	B	603	P5S	C3-O16-P12-O13
2	B	603	P5S	C3-O16-P12-O15
3	A	503	LBN	C1-O1-P1-O2
3	A	508	LBN	C1-O1-P1-O2
3	A	508	LBN	C1-O1-P1-O3
3	A	508	LBN	N1-C6-C9-O2
3	B	601	LBN	C1-O1-P1-O2
3	B	601	LBN	C1-O1-P1-O3
3	B	601	LBN	N1-C6-C9-O2
3	B	604	LBN	C1-O1-P1-O2
4	A	504	A1AIS	C21-O22-P23-O24
4	A	504	A1AIS	C21-O22-P23-O26
4	A	504	A1AIS	C41-C39-O38-C20
4	B	605	A1AIS	C21-O22-P23-O24
4	B	605	A1AIS	C21-O22-P23-O26
4	B	605	A1AIS	C41-C39-O38-C20
5	A	505	6OU	C21-O22-P23-O24
5	A	505	6OU	C21-O22-P23-O26
5	A	505	6OU	C27-O26-P23-O22
5	A	505	6OU	C27-O26-P23-O25
5	A	505	6OU	O26-C27-C28-N29
5	A	505	6OU	O32-C31-O30-C20
5	A	505	6OU	C33-C31-O30-C20
5	B	606	6OU	C21-O22-P23-O24
5	B	606	6OU	C21-O22-P23-O26
5	B	606	6OU	C27-O26-P23-O22
5	B	606	6OU	C27-O26-P23-O25
5	B	606	6OU	O26-C27-C28-N29
5	B	606	6OU	O32-C31-O30-C20
5	B	606	6OU	C33-C31-O30-C20
7	A	507	A1AIT	N33-C34-C35-C38
7	B	608	A1AIT	N33-C34-C35-C38
4	A	504	A1AIS	O40-C39-O38-C20
4	B	605	A1AIS	O40-C39-O38-C20
3	A	508	LBN	C26-C25-O5-C3

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Mol	Chain	Res	Type	Atoms
3	B	601	LBN	C26-C25-O5-C3
2	A	502	P5S	C20-C17-O19-C1
2	B	603	P5S	C20-C17-O19-C1
2	A	501	P5S	C39-C38-O37-C2
2	B	602	P5S	C39-C38-O37-C2
3	A	508	LBN	C35-C34-O7-C2
3	B	601	LBN	C35-C34-O7-C2
3	A	508	LBN	O6-C25-O5-C3
3	B	601	LBN	O6-C25-O5-C3
2	A	502	P5S	O18-C17-O19-C1
2	B	603	P5S	O18-C17-O19-C1
2	A	501	P5S	O47-C38-O37-C2
2	B	602	P5S	O47-C38-O37-C2
2	A	501	P5S	C20-C17-O19-C1
2	B	602	P5S	C20-C17-O19-C1
4	A	504	A1AIS	C44-C45-C46-C47
4	B	605	A1AIS	C44-C45-C46-C47
3	A	508	LBN	O8-C34-O7-C2
3	B	601	LBN	O8-C34-O7-C2
5	A	505	6OU	O30-C20-C21-O22
5	B	606	6OU	O30-C20-C21-O22
5	A	505	6OU	C13-C14-C15-C16
5	B	606	6OU	C13-C14-C15-C16
3	A	508	LBN	C25-C26-C27-C28
3	B	601	LBN	C25-C26-C27-C28
4	A	504	A1AIS	C11-C12-C13-C14
4	B	605	A1AIS	C11-C12-C13-C14
2	A	501	P5S	O18-C17-O19-C1
2	B	602	P5S	O18-C17-O19-C1
4	A	504	A1AIS	C39-C41-C42-C43
4	B	605	A1AIS	C39-C41-C42-C43
2	A	501	P5S	C17-C20-C21-C22
2	B	602	P5S	C17-C20-C21-C22
3	A	503	LBN	C25-C26-C27-C28
3	B	604	LBN	C25-C26-C27-C28
2	A	502	P5S	C39-C38-O37-C2
2	B	603	P5S	C39-C38-O37-C2
3	A	508	LBN	C34-C35-C36-C37
3	B	601	LBN	C34-C35-C36-C37
3	A	503	LBN	C26-C25-O5-C3
3	B	604	LBN	C26-C25-O5-C3
2	A	502	P5S	O47-C38-O37-C2

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Mol	Chain	Res	Type	Atoms
2	B	603	P5S	O47-C38-O37-C2
3	A	503	LBN	C35-C36-C37-C38
3	B	604	LBN	C35-C36-C37-C38
3	A	503	LBN	C26-C27-C28-C29
3	B	604	LBN	C26-C27-C28-C29
3	A	508	LBN	C30-C31-C32-C33
3	B	601	LBN	C30-C31-C32-C33
3	A	503	LBN	O6-C25-O5-C3
3	B	604	LBN	O6-C25-O5-C3
5	A	505	6OU	C08-C09-C10-C11
5	B	606	6OU	C08-C09-C10-C11
3	A	508	LBN	C27-C28-C29-C30
3	B	601	LBN	C27-C28-C29-C30
3	A	508	LBN	C32-C33-C4-C7
3	B	601	LBN	C32-C33-C4-C7
3	A	503	LBN	C35-C34-O7-C2
3	B	604	LBN	C35-C34-O7-C2
2	A	502	P5S	C39-C40-C41-C42
2	B	603	P5S	C39-C40-C41-C42
2	B	602	P5S	C40-C41-C42-C43
2	A	501	P5S	C40-C41-C42-C43
3	A	508	LBN	C29-C30-C31-C32
3	B	601	LBN	C29-C30-C31-C32
5	B	606	6OU	C12-C13-C14-C15
2	A	501	P5S	C28-C29-C30-C31
2	B	602	P5S	C28-C29-C30-C31
5	A	505	6OU	C12-C13-C14-C15
3	A	503	LBN	C9-C6-N1-C12
3	A	503	LBN	C9-C6-N1-C15
3	B	604	LBN	C9-C6-N1-C12
3	B	604	LBN	C9-C6-N1-C15
3	A	503	LBN	O8-C34-O7-C2
3	A	503	LBN	C28-C29-C30-C31
3	B	604	LBN	C28-C29-C30-C31
3	A	503	LBN	O7-C2-C3-O5
3	B	604	LBN	O7-C2-C3-O5
5	A	505	6OU	C41-C42-C43-C44
5	B	606	6OU	C41-C42-C43-C44
3	B	604	LBN	O8-C34-O7-C2
4	A	504	A1AIS	C15-C16-O18-C19
4	B	605	A1AIS	C15-C16-O18-C19
5	A	505	6OU	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
5	B	606	6OU	C36-C37-C38-C39
3	A	503	LBN	C10-C13-C16-C19
5	A	505	6OU	C37-C38-C39-C40
5	B	606	6OU	C37-C38-C39-C40
3	B	604	LBN	C10-C13-C16-C19
3	A	508	LBN	O1-C1-C2-C3
3	B	601	LBN	O1-C1-C2-C3
3	A	503	LBN	C30-C31-C32-C33
3	B	604	LBN	C30-C31-C32-C33
2	A	501	P5S	C43-C44-C45-C46
2	B	602	P5S	C43-C44-C45-C46
2	A	501	P5S	O19-C1-C2-C3
2	A	502	P5S	O19-C1-C2-C3
2	B	602	P5S	O19-C1-C2-C3
2	B	603	P5S	O19-C1-C2-C3
3	A	503	LBN	C29-C30-C31-C32
3	B	604	LBN	C29-C30-C31-C32
5	A	505	6OU	C11-C12-C13-C14
5	B	606	6OU	C11-C12-C13-C14
3	A	503	LBN	C9-C6-N1-C18
3	B	604	LBN	C9-C6-N1-C18
4	A	504	A1AIS	C42-C43-C44-C45
4	B	605	A1AIS	C42-C43-C44-C45
4	A	504	A1AIS	O17-C16-O18-C19
3	B	601	LBN	C31-C32-C33-C4
3	A	508	LBN	C31-C32-C33-C4
3	A	503	LBN	C14-C11-C8-C5
3	B	604	LBN	C14-C11-C8-C5
4	B	605	A1AIS	O17-C16-O18-C19
2	A	501	P5S	C23-C24-C25-C26
2	B	602	P5S	C23-C24-C25-C26
2	A	501	P5S	C30-C31-C32-C33
2	B	602	P5S	C30-C31-C32-C33
3	A	508	LBN	C13-C10-C7-C4
3	B	601	LBN	C13-C10-C7-C4
2	A	501	P5S	C22-C23-C24-C25
2	B	602	P5S	C22-C23-C24-C25
2	A	502	P5S	C1-C2-C3-O16
2	B	603	P5S	C1-C2-C3-O16
5	A	505	6OU	C19-C20-C21-O22
5	B	606	6OU	C19-C20-C21-O22
4	A	504	A1AIS	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
4	B	605	A1AIS	C41-C42-C43-C44
3	A	503	LBN	C1-C2-C3-O5
3	B	604	LBN	C1-C2-C3-O5
4	A	504	A1AIS	O18-C19-C20-C21
4	B	605	A1AIS	O18-C19-C20-C21
4	A	504	A1AIS	O38-C20-C21-O22
4	B	605	A1AIS	O38-C20-C21-O22
2	A	501	P5S	O19-C1-C2-O37
2	A	502	P5S	O19-C1-C2-O37
2	B	602	P5S	O19-C1-C2-O37
2	B	603	P5S	O19-C1-C2-O37
4	A	504	A1AIS	O18-C19-C20-O38
4	B	605	A1AIS	O18-C19-C20-O38
3	A	508	LBN	C28-C29-C30-C31
3	B	601	LBN	C28-C29-C30-C31
5	A	505	6OU	C15-C16-O18-C19
5	B	606	6OU	C15-C16-O18-C19
2	B	602	P5S	C39-C40-C41-C42
2	A	501	P5S	C39-C40-C41-C42
3	A	503	LBN	C27-C28-C29-C30
3	B	604	LBN	C27-C28-C29-C30
3	A	508	LBN	C35-C36-C37-C38
3	B	601	LBN	C35-C36-C37-C38
3	A	503	LBN	C6-C9-O2-P1
3	B	604	LBN	C6-C9-O2-P1
2	A	501	P5S	N-CA-CB-OG
2	B	602	P5S	N-CA-CB-OG
5	A	505	6OU	O17-C16-O18-C19
5	B	606	6OU	O17-C16-O18-C19
4	A	504	A1AIS	C19-C20-C21-O22
4	B	605	A1AIS	C19-C20-C21-O22
7	A	507	A1AIT	C35-C34-N33-C39
7	B	608	A1AIT	C35-C34-N33-C39
2	A	502	P5S	O37-C2-C3-O16
2	B	603	P5S	O37-C2-C3-O16
2	A	502	P5S	C20-C21-C22-C23
5	A	505	6OU	C35-C36-C37-C38
5	B	606	6OU	C35-C36-C37-C38
2	A	501	P5S	CB-OG-P12-O13
2	A	501	P5S	C3-O16-P12-OG
2	A	501	P5S	C3-O16-P12-O13
2	A	501	P5S	C3-O16-P12-O15

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Mol	Chain	Res	Type	Atoms
2	B	602	P5S	CB-OG-P12-O13
2	B	602	P5S	C3-O16-P12-OG
2	B	602	P5S	C3-O16-P12-O13
2	B	602	P5S	C3-O16-P12-O15
3	A	503	LBN	C1-O1-P1-O4
3	A	503	LBN	C9-O2-P1-O1
3	A	503	LBN	C9-O2-P1-O3
3	A	503	LBN	C9-O2-P1-O4
3	A	508	LBN	C1-O1-P1-O4
3	B	601	LBN	C1-O1-P1-O4
3	B	604	LBN	C1-O1-P1-O4
3	B	604	LBN	C9-O2-P1-O1
3	B	604	LBN	C9-O2-P1-O3
3	B	604	LBN	C9-O2-P1-O4
4	A	504	A1AIS	C21-O22-P23-O25
4	B	605	A1AIS	C21-O22-P23-O25
5	A	505	6OU	C21-O22-P23-O25
5	B	606	6OU	C21-O22-P23-O25
2	B	603	P5S	C20-C21-C22-C23
3	A	508	LBN	C2-C1-O1-P1
3	B	601	LBN	C2-C1-O1-P1
5	A	505	6OU	C20-C21-O22-P23
5	B	606	6OU	C20-C21-O22-P23
2	A	501	P5S	C3-C2-O37-C38
2	B	602	P5S	C3-C2-O37-C38
3	A	508	LBN	O1-C1-C2-O7
3	B	601	LBN	O1-C1-C2-O7
5	A	505	6OU	C09-C10-C11-C12
5	B	606	6OU	C09-C10-C11-C12
3	A	503	LBN	C39-C40-C41-C42
3	B	604	LBN	C39-C40-C41-C42
2	A	501	P5S	C27-C28-C29-C30
2	B	602	P5S	C27-C28-C29-C30
2	A	502	P5S	C38-C39-C40-C41
2	B	603	P5S	C38-C39-C40-C41
3	A	503	LBN	C2-C1-O1-P1
3	B	604	LBN	C2-C1-O1-P1
2	B	602	P5S	C44-C45-C46-C48
2	A	501	P5S	C44-C45-C46-C48
4	A	504	A1AIS	C20-C21-O22-P23
4	B	605	A1AIS	C20-C21-O22-P23
2	A	502	P5S	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
2	B	603	P5S	C40-C41-C42-C43
2	A	502	P5S	C21-C22-C23-C24
2	B	603	P5S	C21-C22-C23-C24
5	A	505	6OU	C40-C41-C42-C43
5	B	606	6OU	C40-C41-C42-C43
3	A	503	LBN	C40-C41-C42-C5
3	B	604	LBN	C40-C41-C42-C5
5	A	505	6OU	C10-C11-C12-C13
5	B	606	6OU	C10-C11-C12-C13
3	A	503	LBN	C42-C5-C8-C11
3	B	604	LBN	C42-C5-C8-C11
2	A	501	P5S	C20-C21-C22-C23
2	B	602	P5S	C20-C21-C22-C23
3	A	503	LBN	C38-C39-C40-C41
3	B	604	LBN	C38-C39-C40-C41
2	A	501	P5S	C38-C39-C40-C41
2	B	602	P5S	C38-C39-C40-C41
3	A	503	LBN	C13-C10-C7-C4
2	A	501	P5S	C1-C2-O37-C38
2	B	602	P5S	C1-C2-O37-C38
3	B	604	LBN	C13-C10-C7-C4
5	A	505	6OU	C07-C08-C09-C10
5	B	606	6OU	C07-C08-C09-C10
2	A	502	P5S	O37-C38-C39-C40
2	B	603	P5S	O37-C38-C39-C40

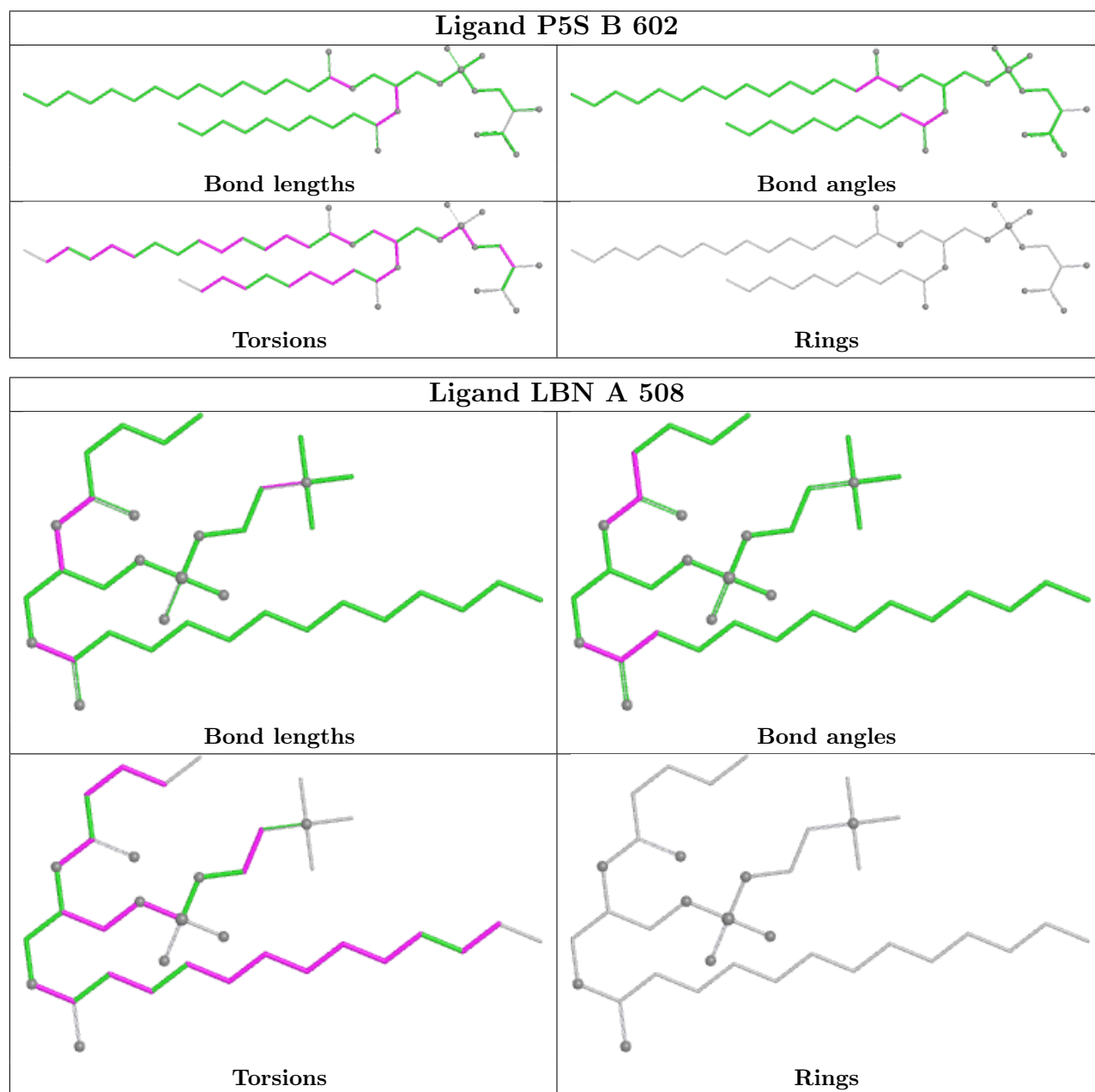
There are no ring outliers.

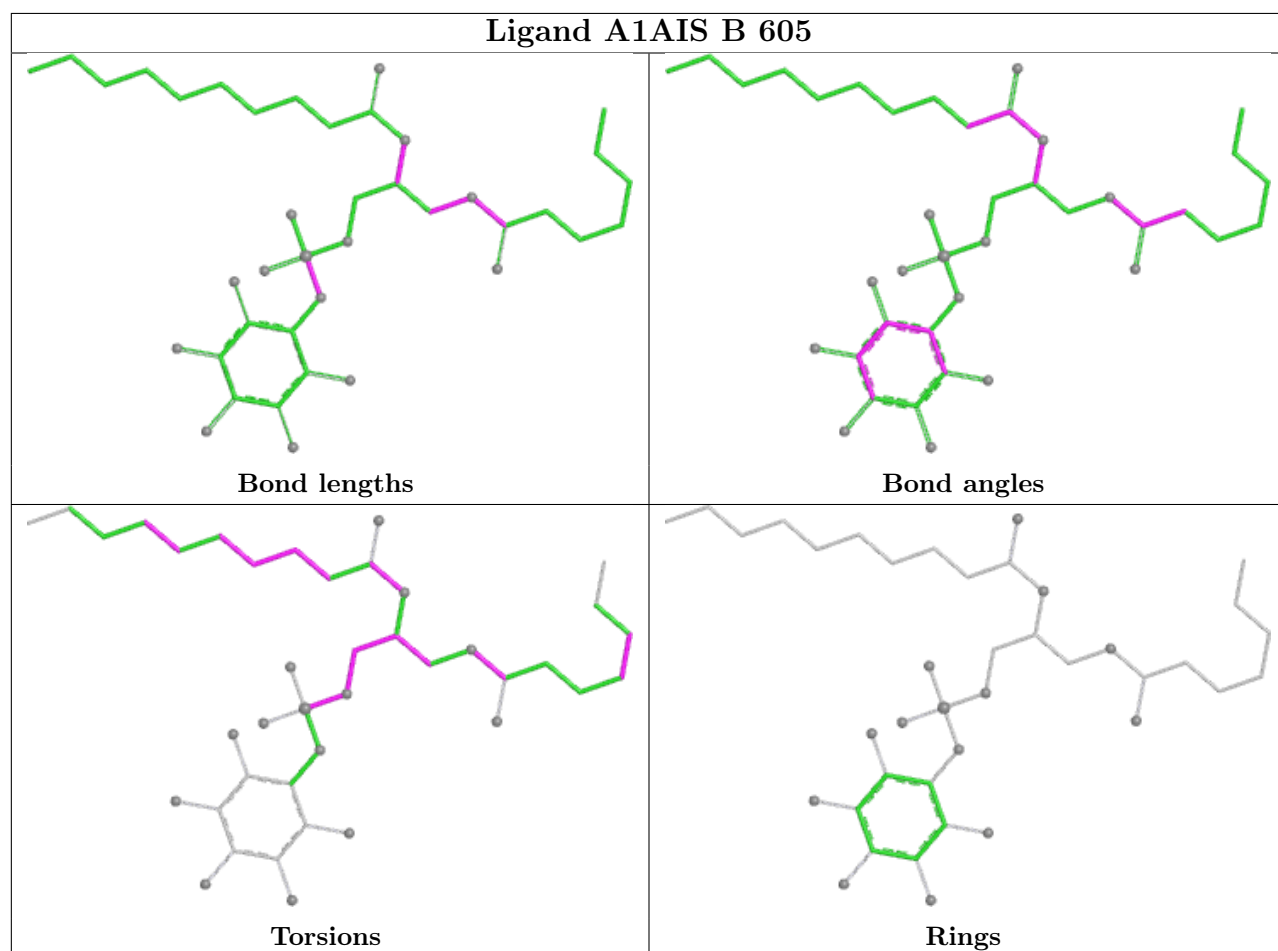
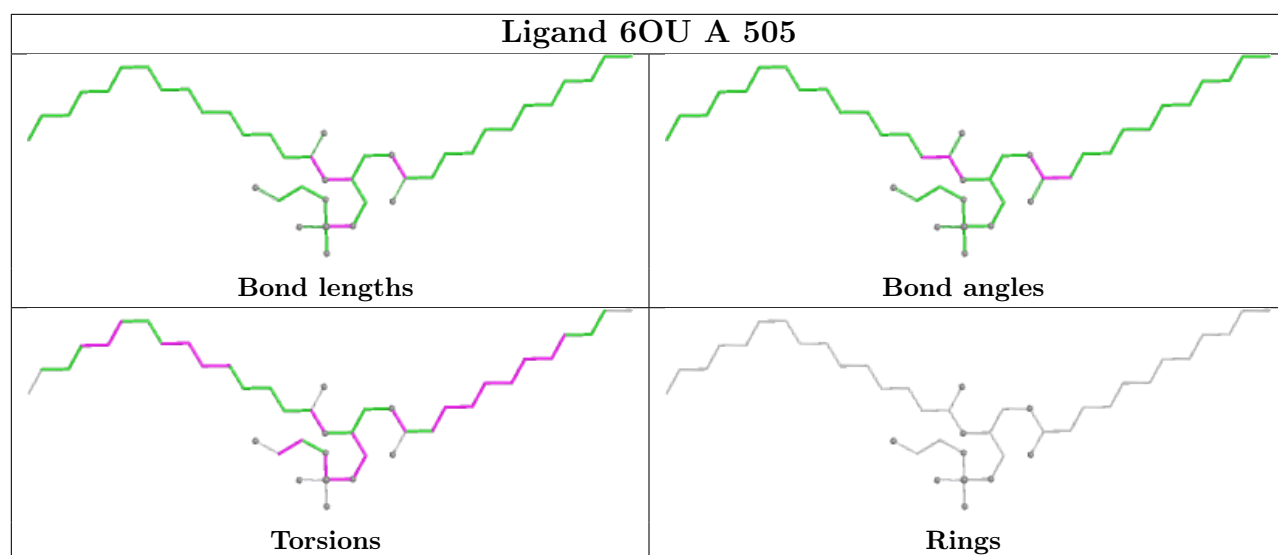
5 monomers are involved in 8 short contacts:

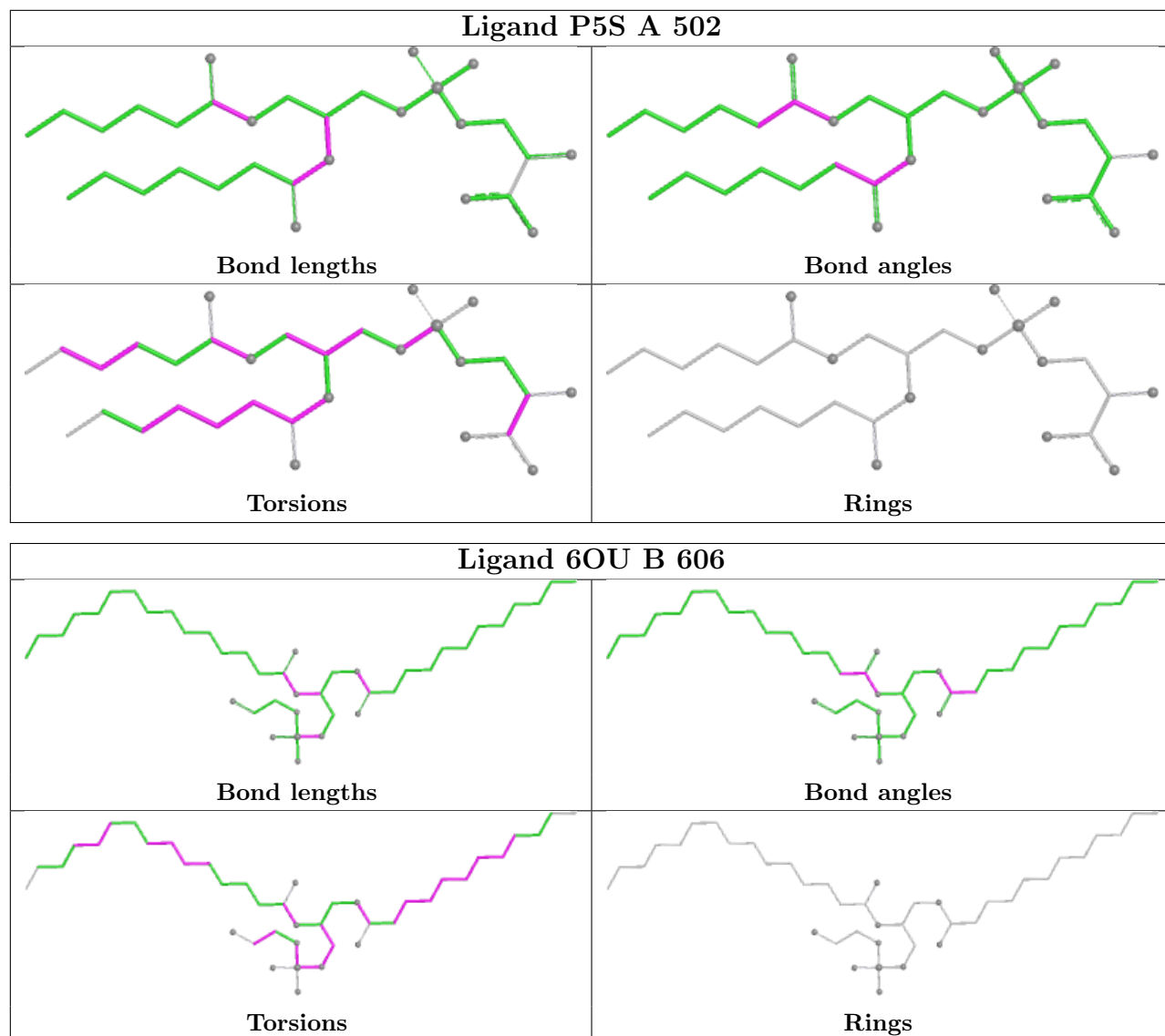
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	6OU	1	0
4	B	605	A1AIS	1	0
2	A	502	P5S	3	0
5	B	606	6OU	1	0
2	B	603	P5S	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

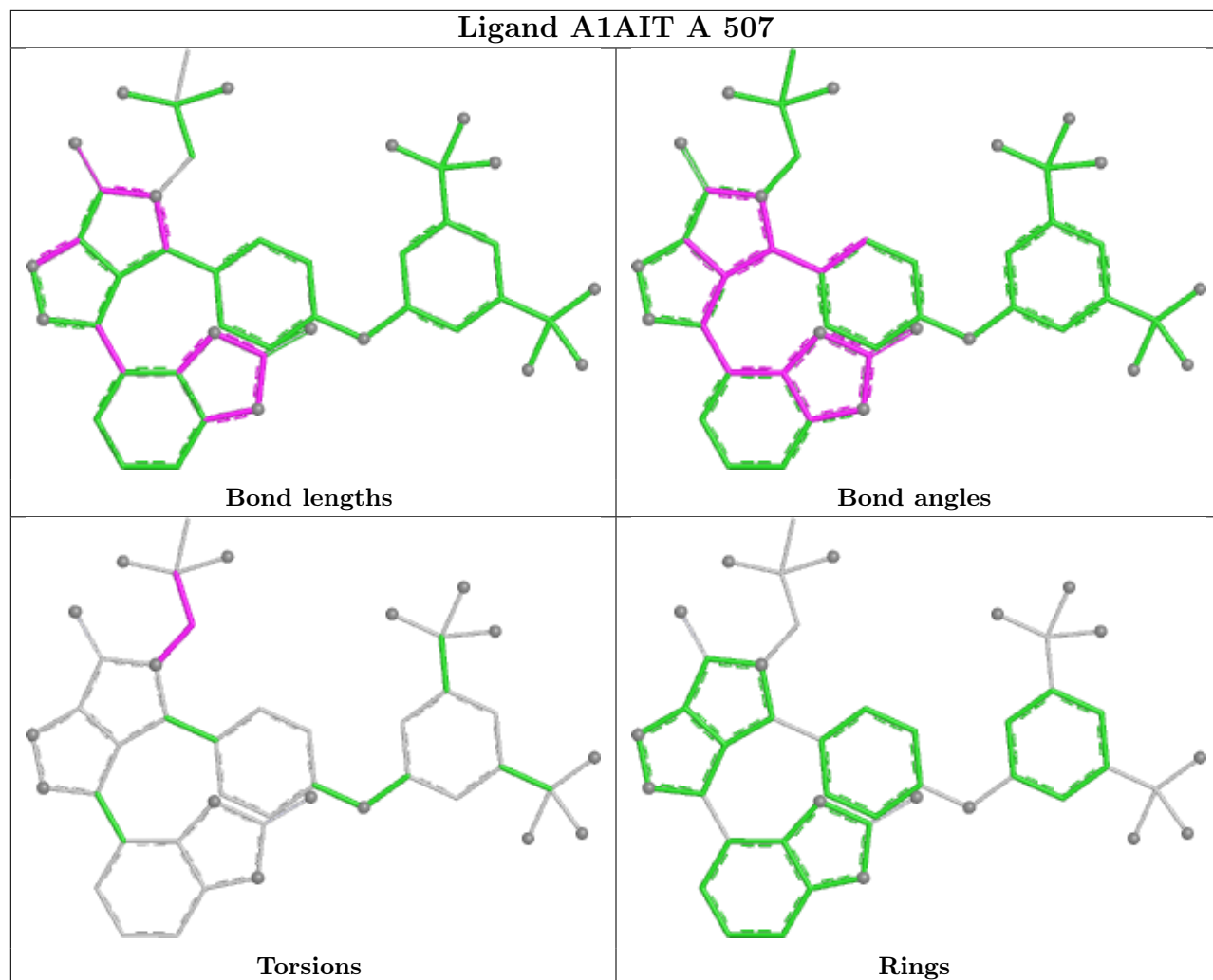
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

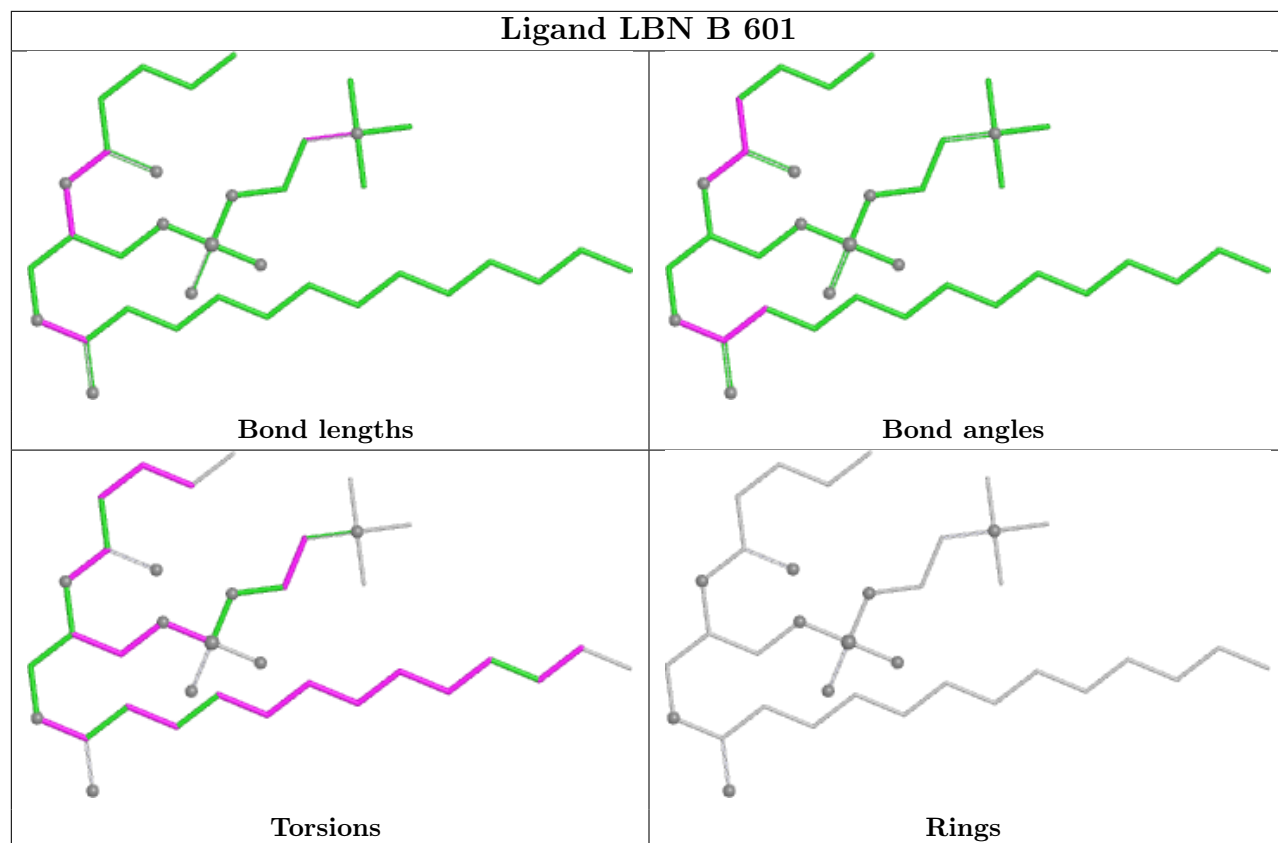




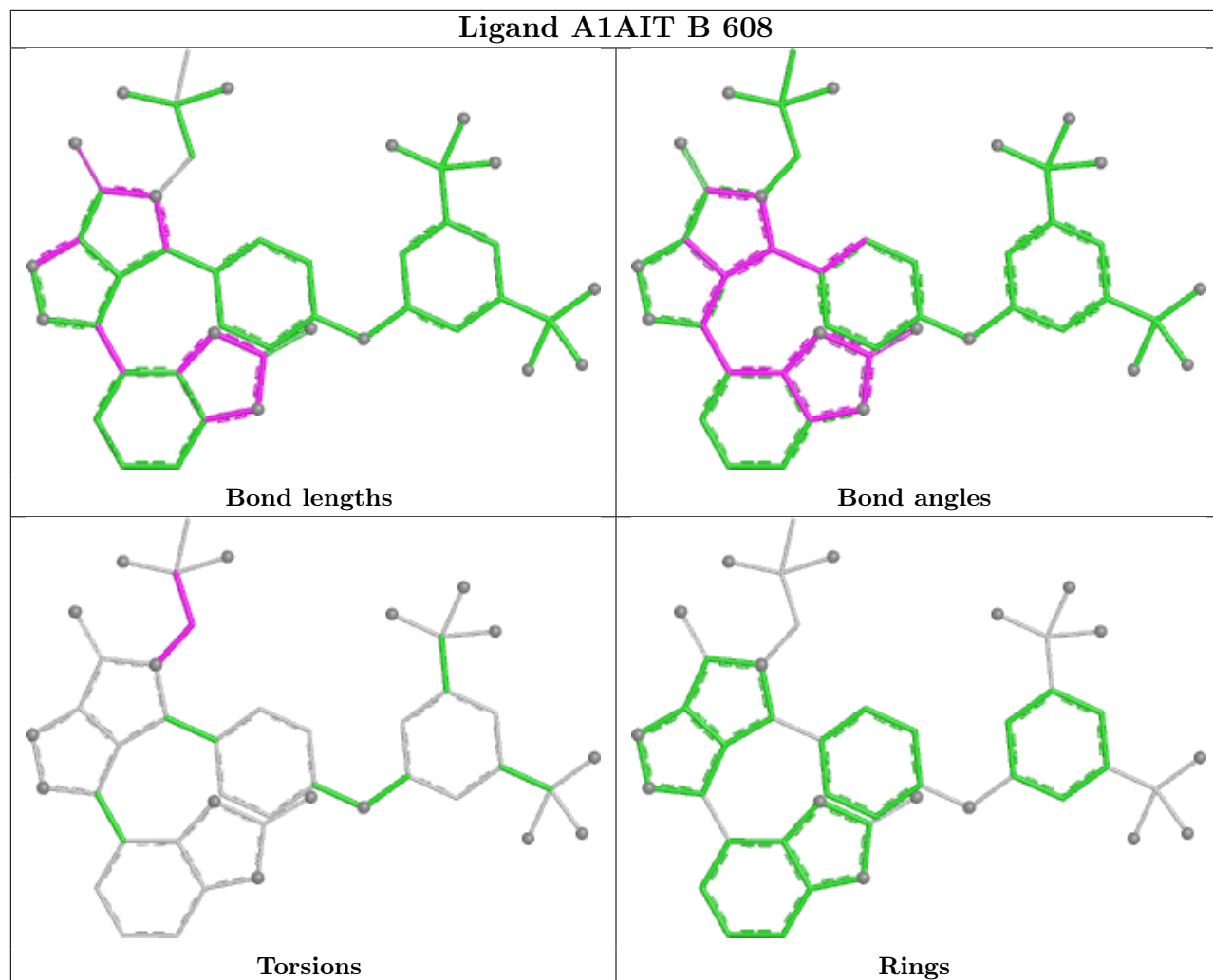


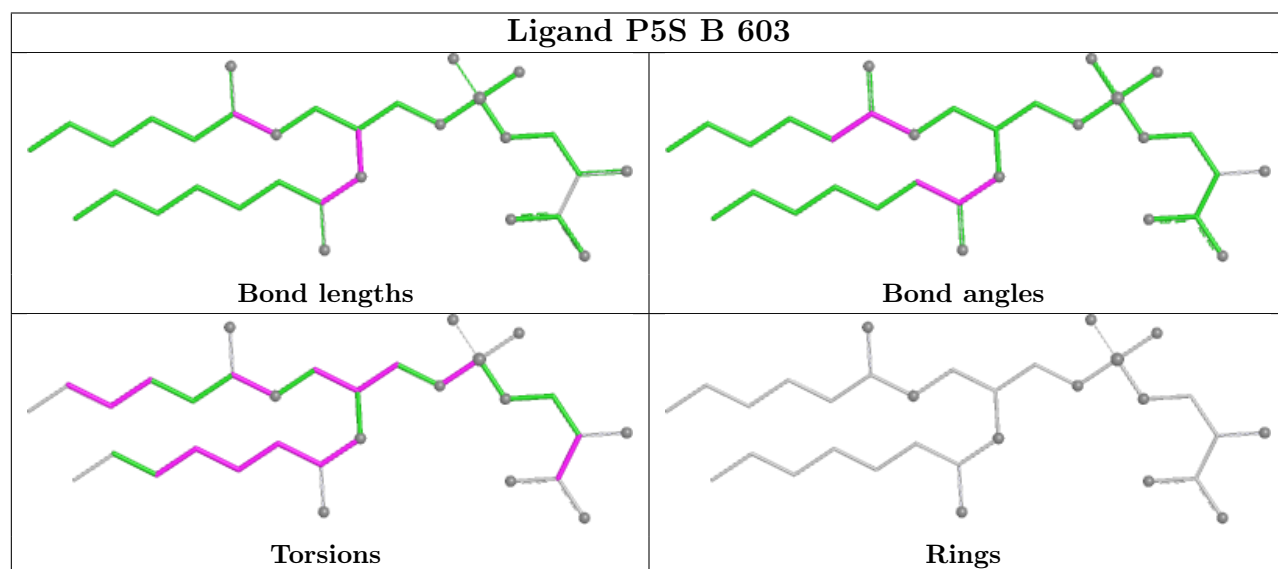
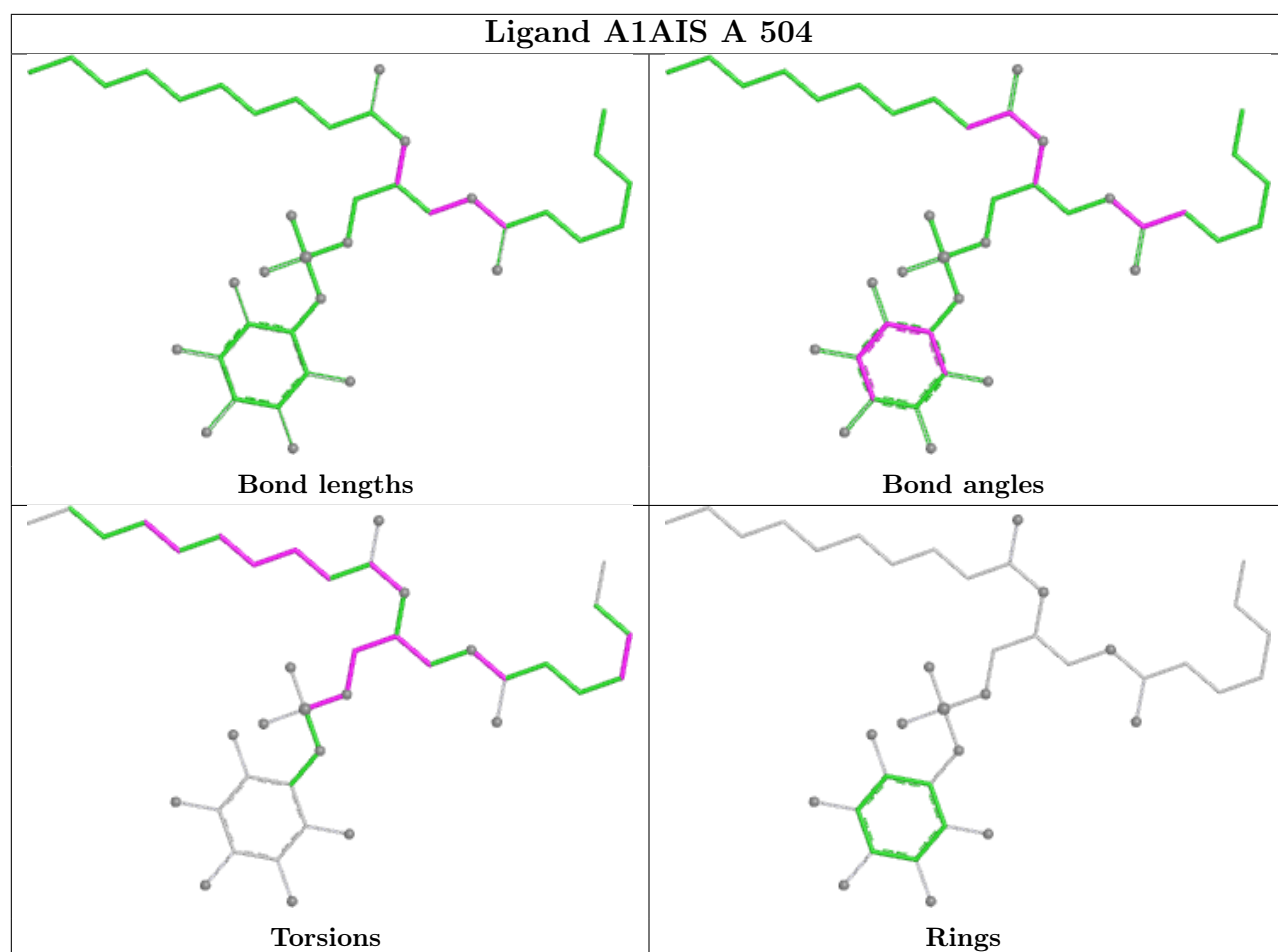
Ligand A1AIT A 507

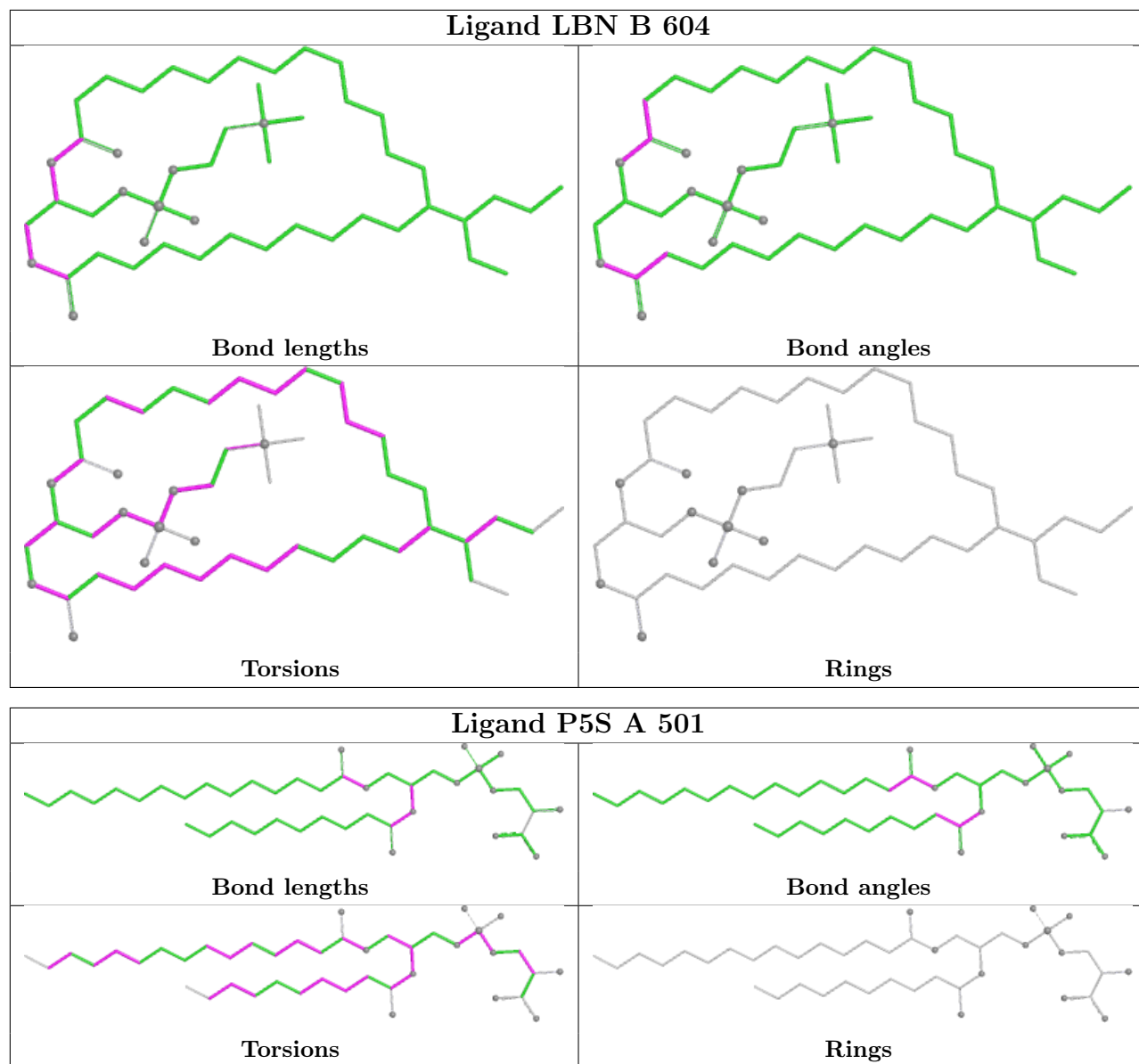


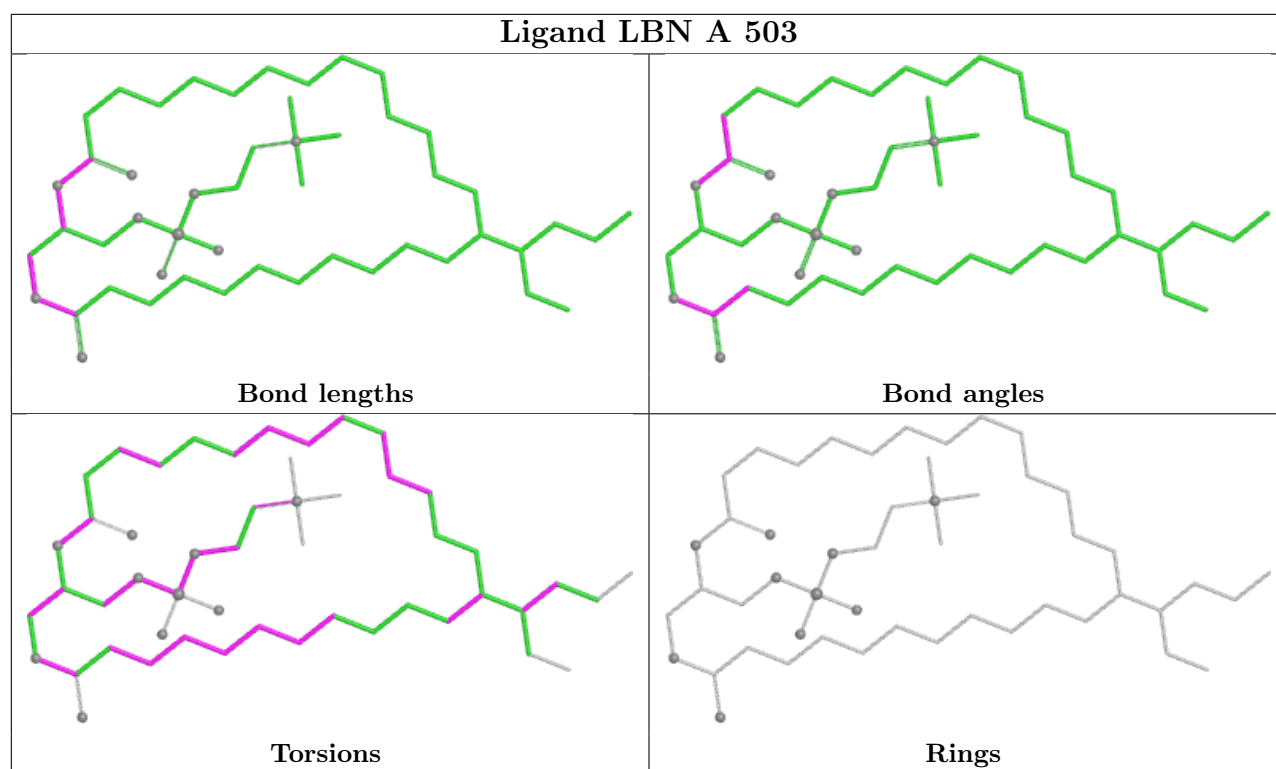


Ligand A1AIT B 608









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

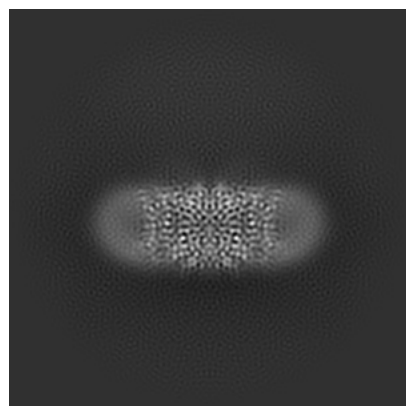
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44180. These allow visual inspection of the internal detail of the map and identification of artifacts.

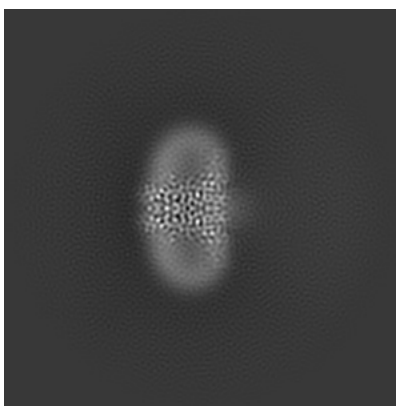
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

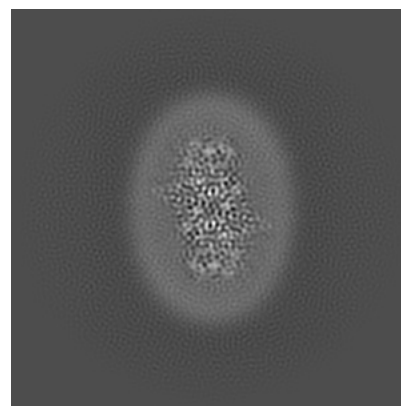
6.1.1 Primary map



X

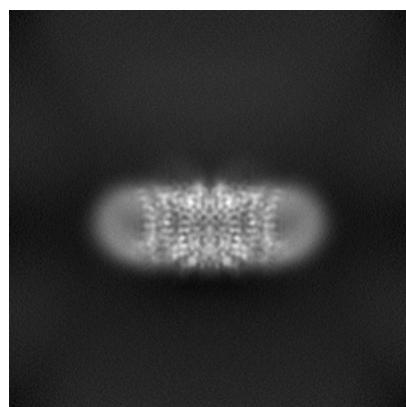


Y

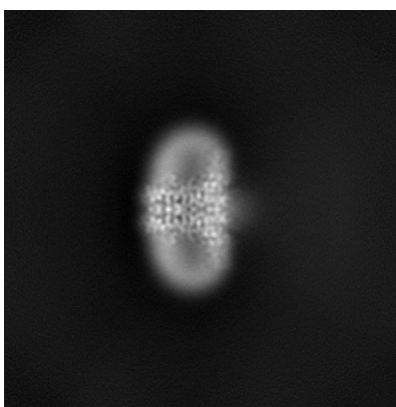


Z

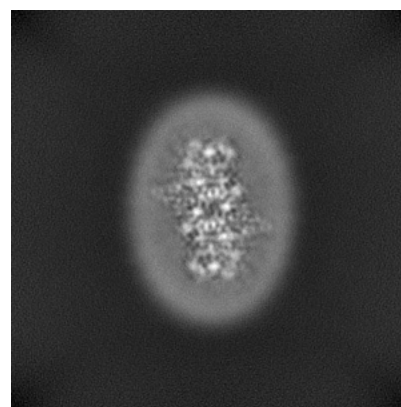
6.1.2 Raw map



X



Y

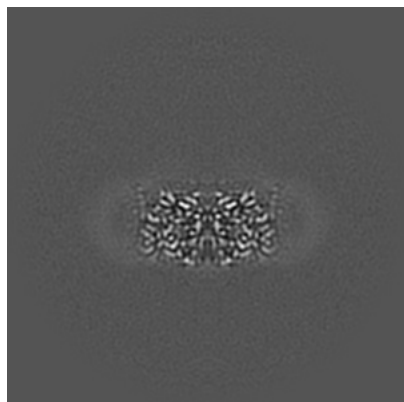


Z

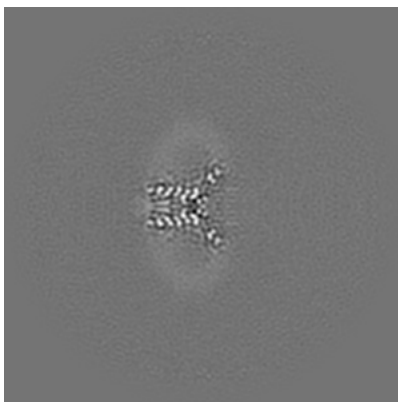
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

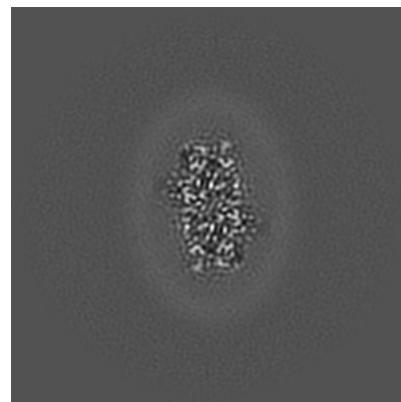
6.2.1 Primary map



X Index: 150

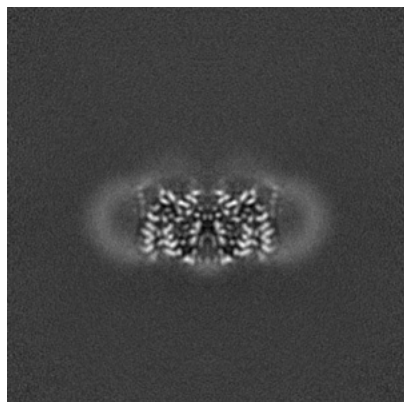


Y Index: 150

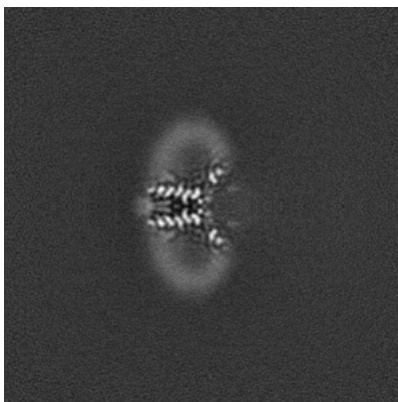


Z Index: 150

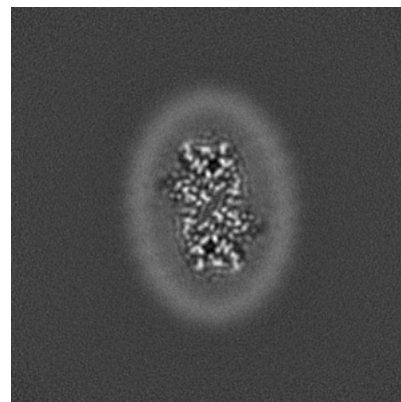
6.2.2 Raw map



X Index: 150



Y Index: 150

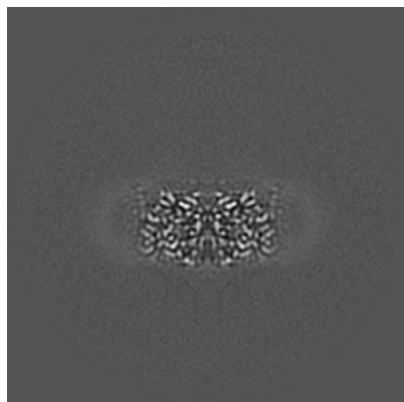


Z Index: 150

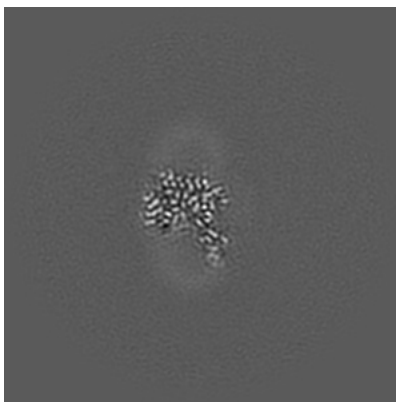
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

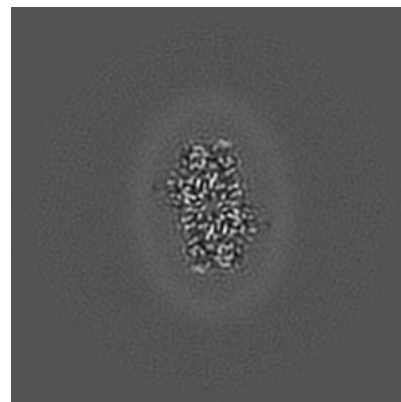
6.3.1 Primary map



X Index: 150

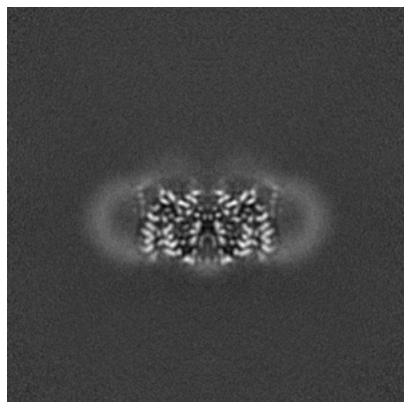


Y Index: 165

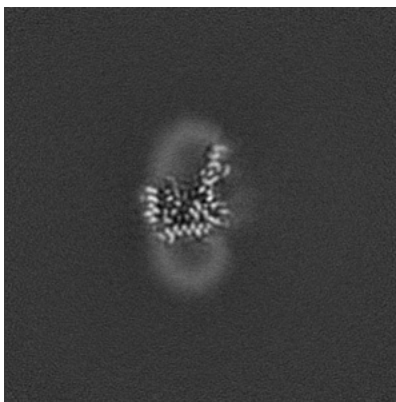


Z Index: 151

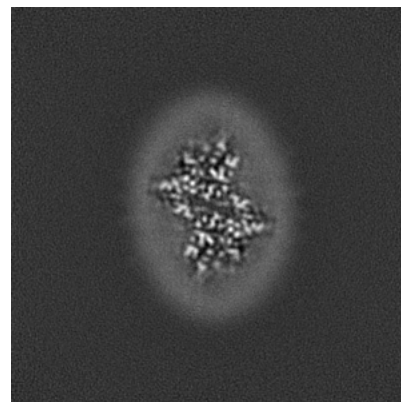
6.3.2 Raw map



X Index: 150



Y Index: 136

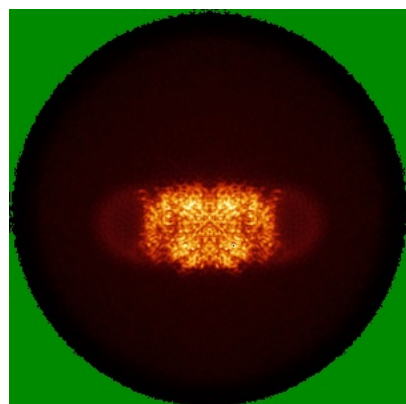


Z Index: 156

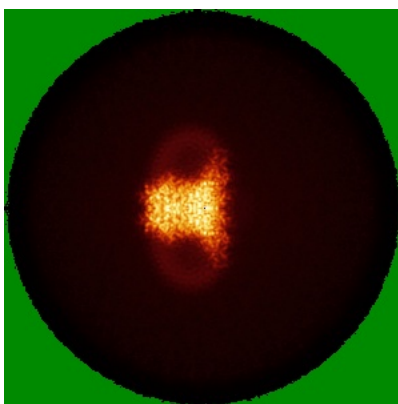
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

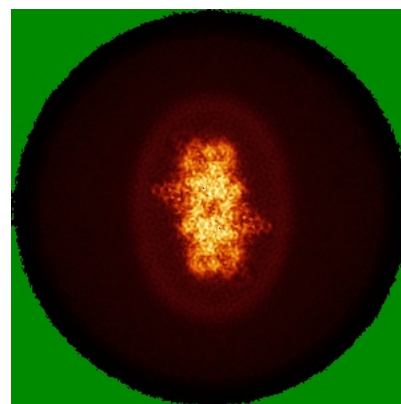
6.4.1 Primary map



X

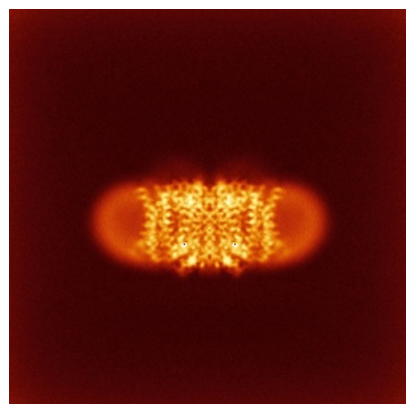


Y

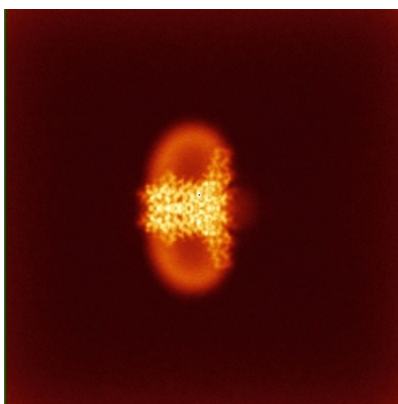


Z

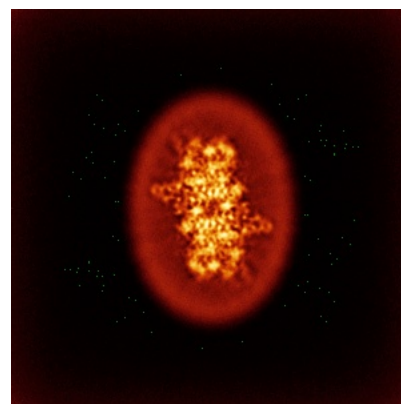
6.4.2 Raw map



X



Y

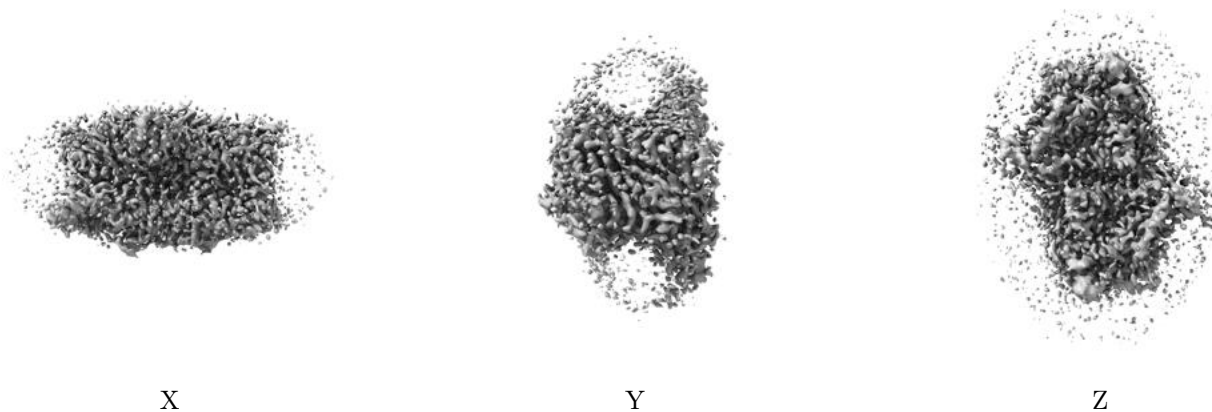


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

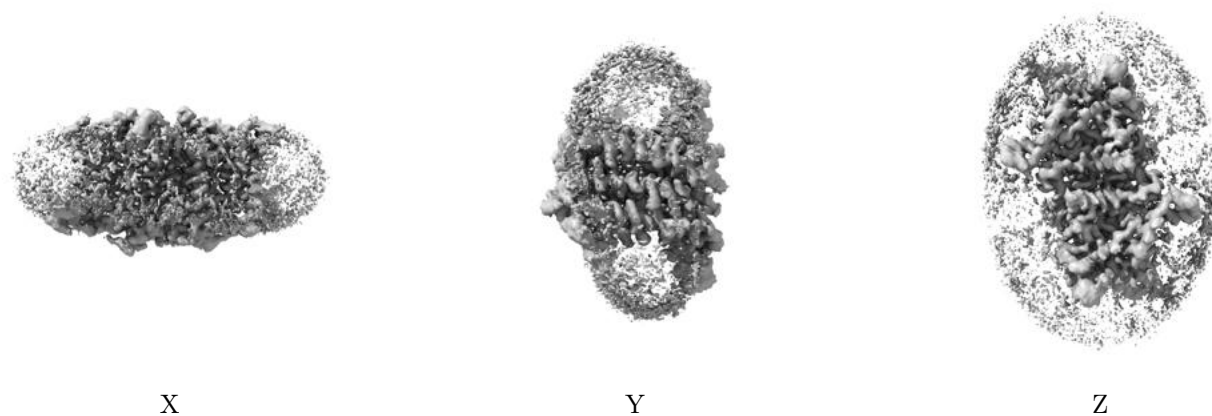
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.312. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

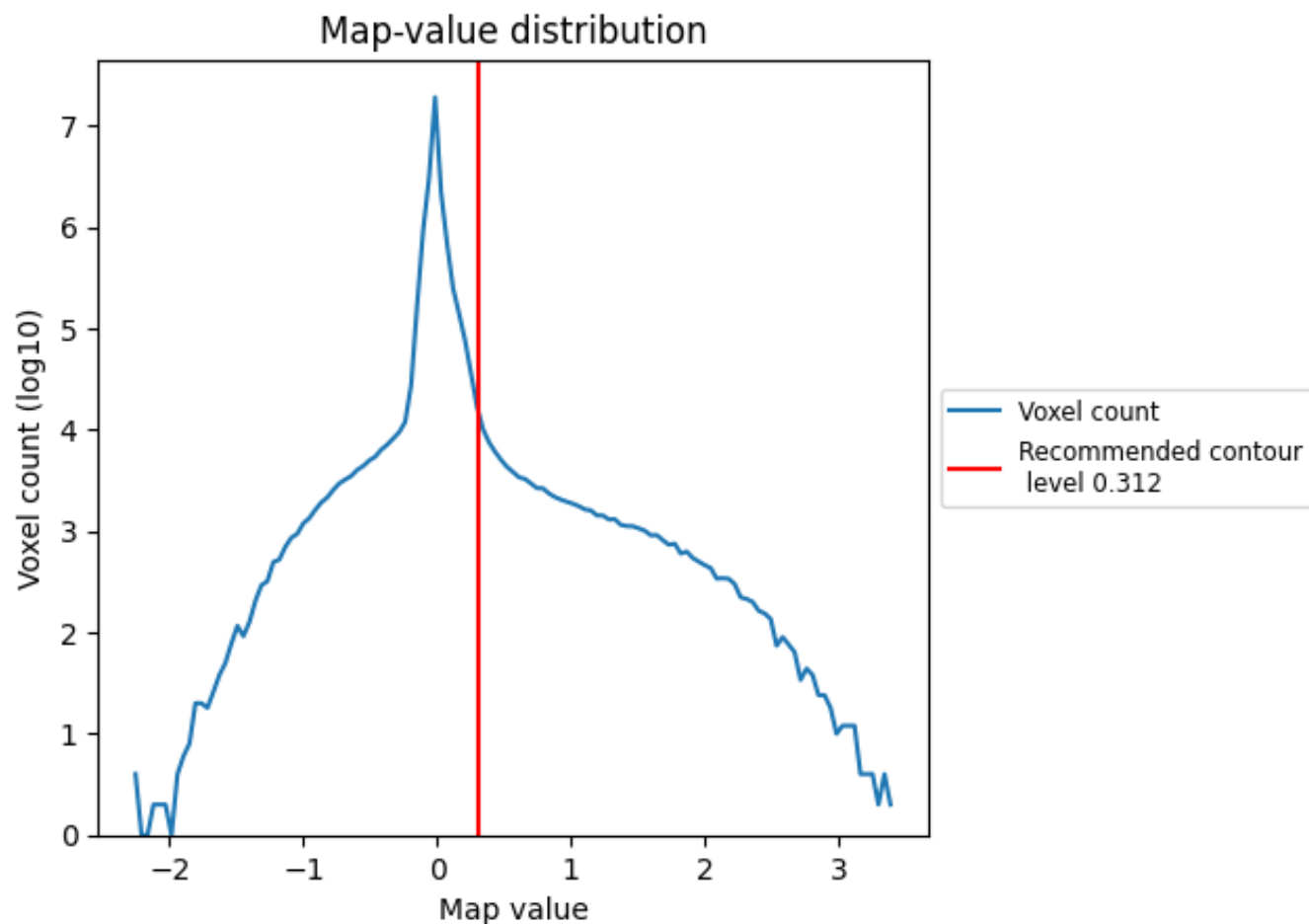
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

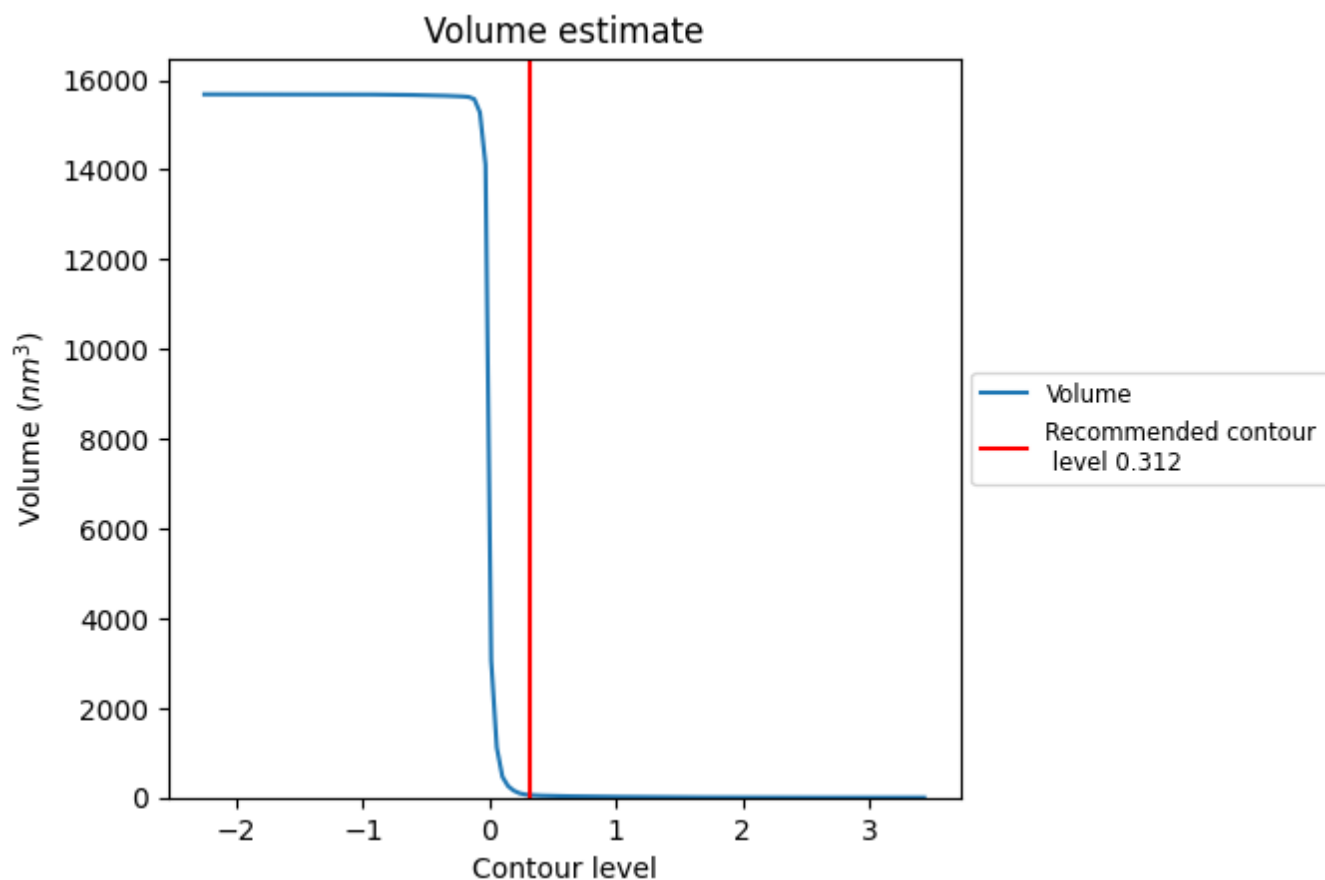
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

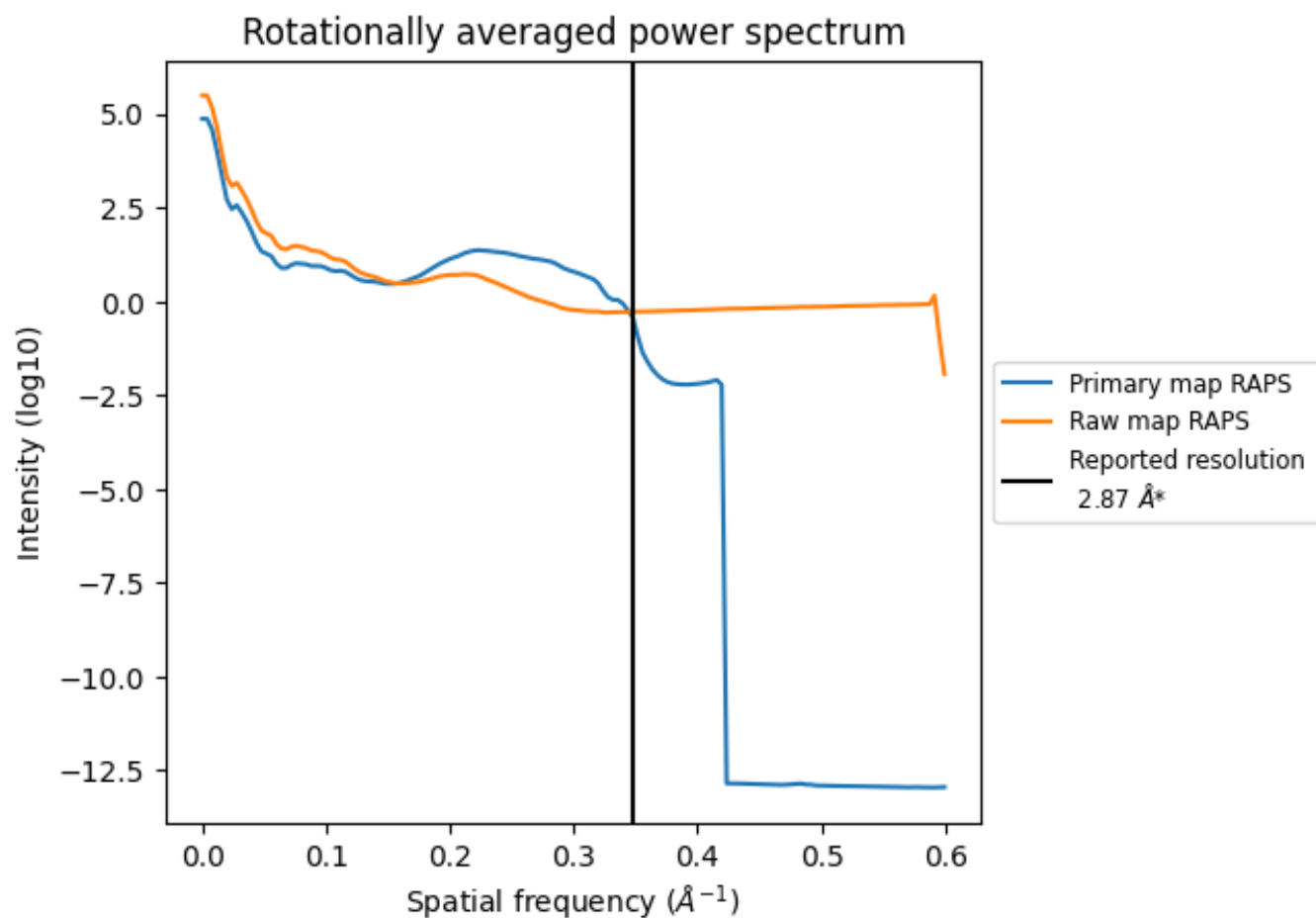
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 58 nm³; this corresponds to an approximate mass of 53 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

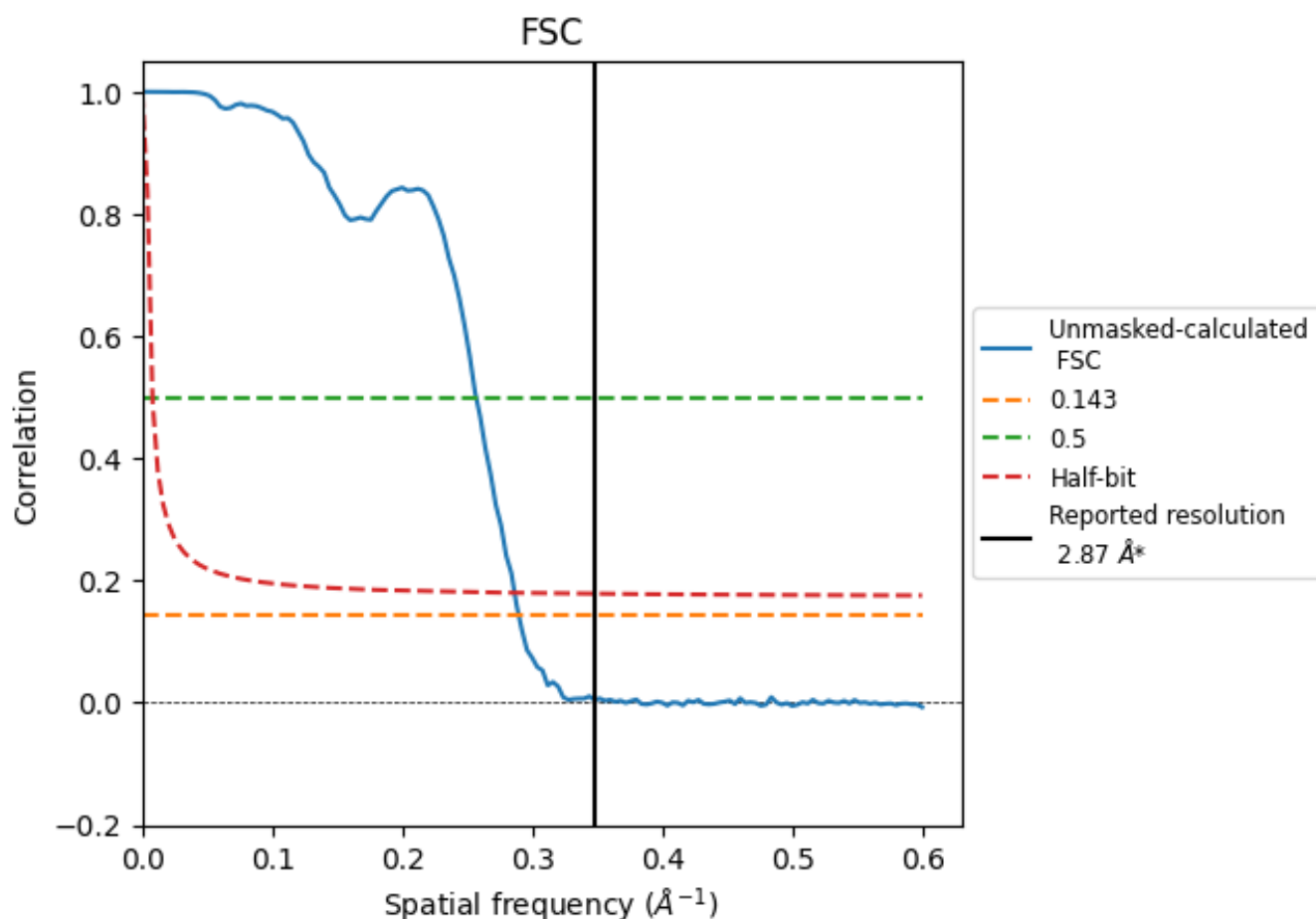


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.348 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

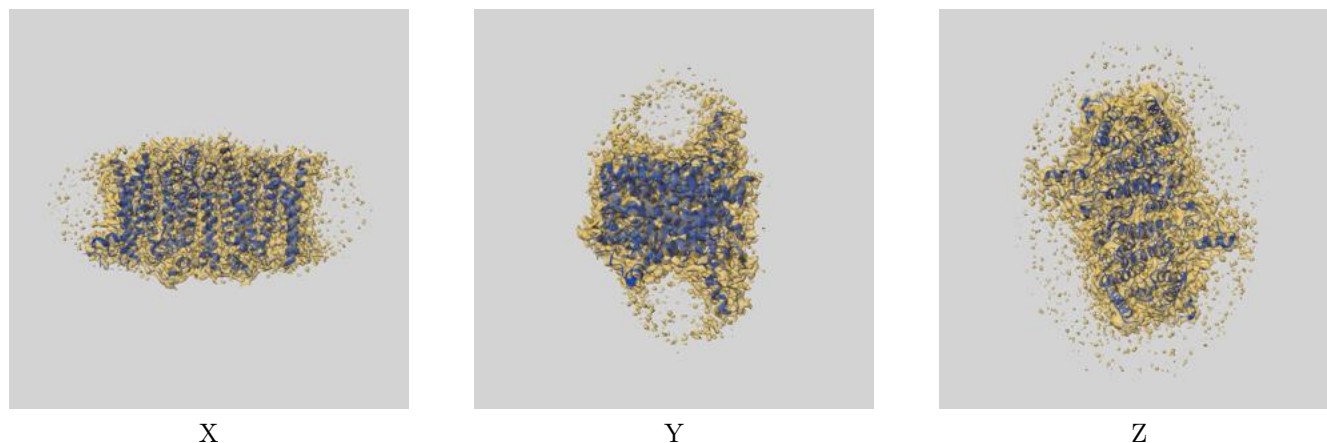
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.46	3.90	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

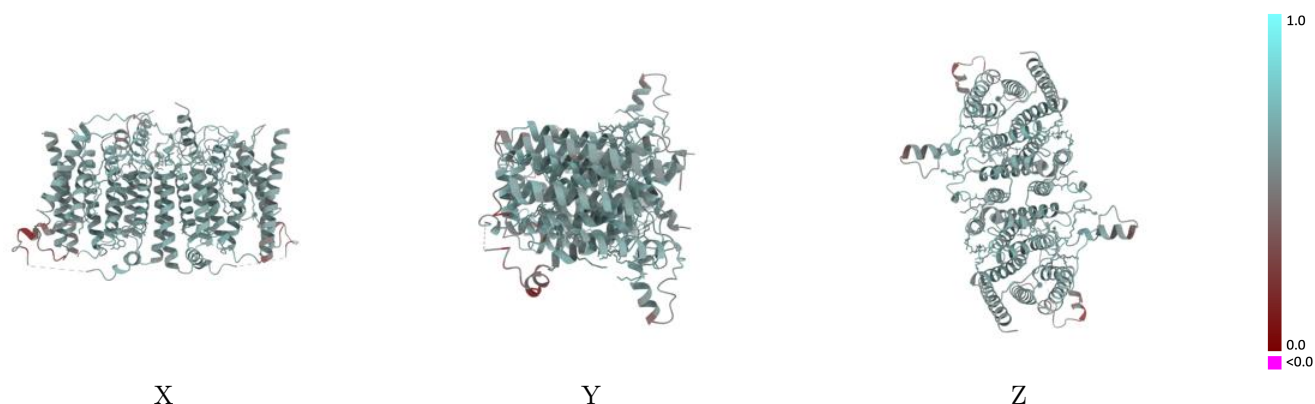
This section contains information regarding the fit between EMDB map EMD-44180 and PDB model 9B4G. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



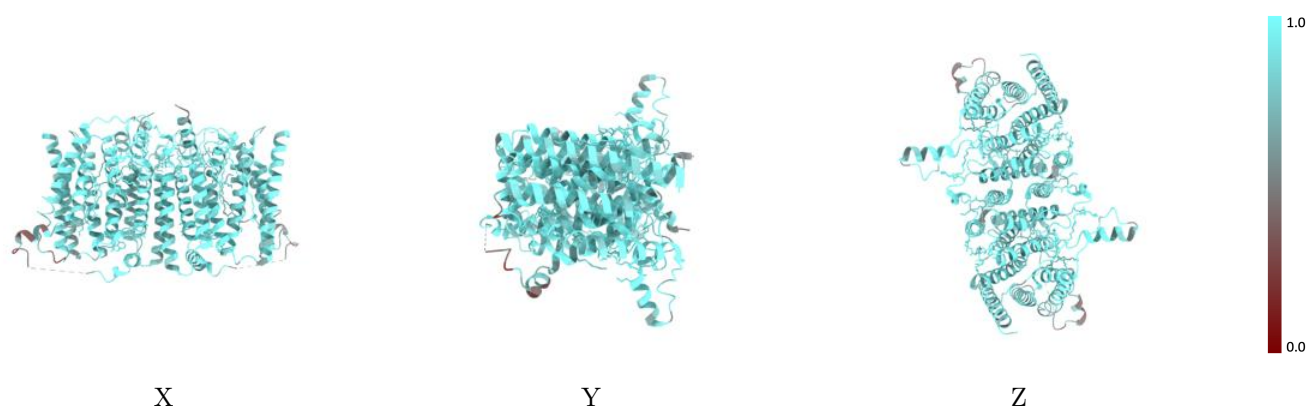
The images above show the 3D surface view of the map at the recommended contour level 0.312 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



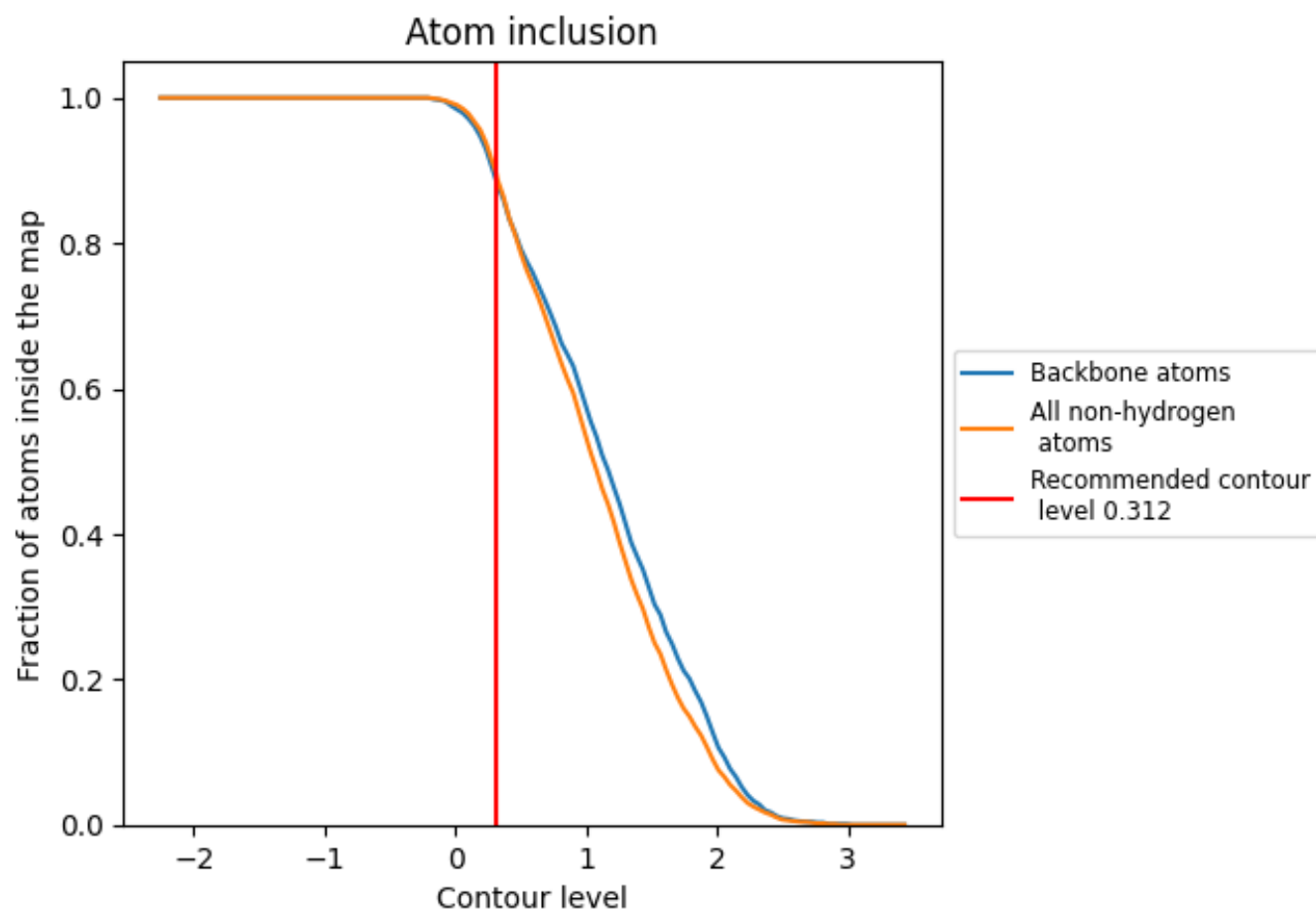
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.312).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.312) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8960	0.5770
A	0.8970	0.5770
B	0.8970	0.5770

